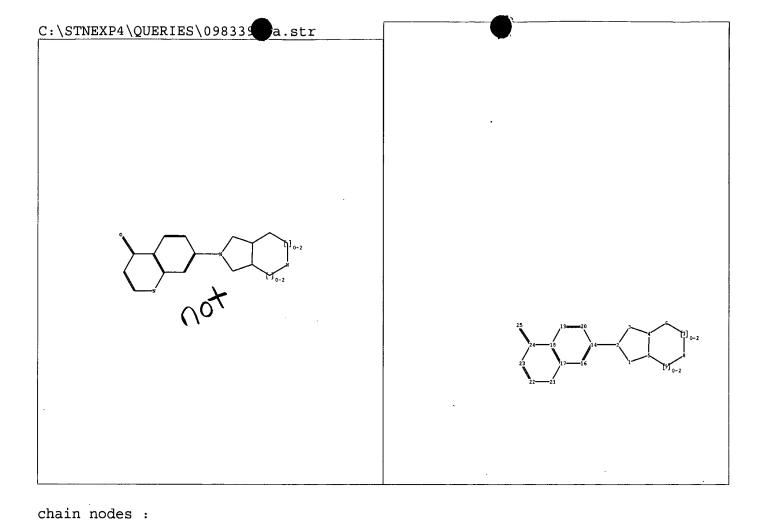


```
ring nodes :
    1 2 3 4 5 6 7 8 9
chain bonds :
    2-14
ring bonds :
    1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9
exact/norm bonds :
    2-14
exact bonds :
    1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9
isolated ring systems :
    containing 1 :

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 14:Atom
```

14



```
25
ring nodes :
   1 2 3 4 5 6 7 8 9 14 16 17 18 19 20 21 22 23 24
chain bonds :
   2-14 24-25
ring bonds :
   1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9 14-16 14-20 16-17
   17-18 17-21 18-19 18-24 19-20 21-22 22-23 23-24
exact/norm bonds :
   2-14 17-21 18-24 21-22 22-23 23-24 24-25
exact bonds :
   1-2 1-5 2-3 3-4 4-5 4-6 5-9 6-7 7-8 8-9
normalized bonds :
   14-16 14-20 16-17 17-18 18-19 19-20
isolated ring systems :
   containing 1 :
Match level :
   1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
   14:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom 22:Atom
   23:Atom 24:Atom 25:CLASS
```

=> d his

(FILE 'HOME' ENTERED AT 16:06:42 ON 11 DEC 2002)

FILE 'REGISTRY' ENTERED AT 16:06:46 ON 11 DEC 2002

L5 STRUCTURE UPLOADED

L6 QUE L5

L7 5 S L6

L8 475 S L6 SSS FUL

FILE 'CAPLUS' ENTERED AT 16:11:45 ON 11 DEC 2002

L9 602 S L8

L10 ANALYZE L9 1- RN HIT : 471 TERMS

FILE 'REGISTRY' ENTERED AT 16:12:27 ON 11 DEC 2002

L11 1 S 151096-09-2/RN L12 1 S 144194-96-7/RN

L13 1 S 186826-86-8/RN

FILE 'REGISTRY' ENTERED AT 16:16:14 ON 11 DEC 2002

L14 STRUCTURE UPLOADED

L15 QUE L14

L16 231 S L15 SUB=L8 FUL

L17 244 S L8 NOT L16

FILE 'CAPLUS' ENTERED AT 16:22:34 ON 11 DEC 2002

L18 28 S L17

=> d 16

L6 HAS NO ANSWERS

L5 STR

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & \\ & & \\$$

Structure attributes must be viewed using STN Express query preparation. L6 $$\tt QUE $\tt ABB=ON $\tt PLU=ON $\tt L5$$

=> d 115

L15 HAS NO ANSWERS

L14 STR

Structure attributes must be viewed using STN Express query preparation. L15 $$\tt QUE \tt ABB=ON \tt PLU=ON \tt L14 \tt$

=> d bib abs hitstr 118 1-28

L11 1 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo- (9CI)

MF C21 H24 F N3 O4

CI COM

Absolute stereochemistry. Rotation (-).

151096-09-2 466 ref.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

ALL ANSWERS HAVE BEEN SCANNED

=> d scan 112

L12 1 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3-Quinolinecarboxylic acid, 8-chloro-1-cyclopropyl-6-fluoro-1,4-dihydro-7[(4as,7as)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-,
monohydrochloride (9CI)

MF C20 H21 Cl F N3 O3 . Cl H

Absolute stereochemistry.

144194-96-7 66 ref

● HCl

ALL ANSWERS HAVE BEEN SCANNED

13 1 ANSWERS REGISTRY COPYRIGHT 2002 ACS

IN 3-Quinolinecarboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-8-methoxy-7[(4as,7as)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-,
monohydrochloride (9CI)

MF C21 H24 F N3 O4 . C1 H

Absolute stereochemistry. Rotation (-).

● HCl

ALL ANSWERS HAVE BEEN SCANNED

186826-86-8 34 reg ıX;

ANSWER 1 OF 28 CAPLUS COPYRIGHT 2002 ACS

2002:835034 CAPLUS

TI Synthesis and Structure-Activity Relationships of Novel 7-Substituted 1,4-Dihydro-4-oxo-1-(2-thiazolyl)-1,8-naphthyridine-3-carboxylic Acids as Antitumor Agents. Part 1

AU Tomita, Kyoji; Tsuzuki, Yasunori; Shibamori, Koh-ichiro; Tashima, Masanori; Kajikawa, Fumie; Sato, Yuji; Kashimoto, Shigeki; Chiba, Katsumi; Hino, Katsuhiko

CS Chemistry Research Laboratories, Dainippon Pharmaceutical Co. Ltd., Osaka, 564-0053, Japan

SO Journal of Medicinal Chemistry (2002), 45(25), 5564-5575 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

GΙ

$$\begin{array}{c|c} & \circ & \\ & & & \\ R & & N & \\ & & N & \\ & & \\ & & & \\ & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

AB Title compds., e.g. I (R = H2NCH2CH2NH, 1-pyrrolidinyl, 3-hydroxy-1-pyrrolidinyl), possess moderate cytotoxic activity. Structure-activity relationships of title compds. were investigated by changing substituents at N-1 and C-7 positions and the core ring structure itself and evaluated the synthesized compds. against several murine and human tumor cell lines. The 2-thiazolyl group at the N-1 position of the naphthyridine structure is the best substituent for antitumor activity and regarding core ring structure, the naphthyridine deriv. is the most active followed by pyridopyrimidine analog. At the C-7 position, aminopyrrolidine derivs. are more effective than other amines or thioether derivs. I (R = 3-amino-4-methoxy-1-pyrrolidinyl, 3-amino-3-methyl-1-pyrrolidinyl, 3-aminopyrrolidinyl) were detd. to be effective in vitro and in vivo antitumor assays, and their activity was comparable to that of etoposide.

IT 475468-86-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and structure-antitumor relationships of naphthyridinecarboxylates)

RN 475468-86-1 CAPLUS

CN INDEX NAME NOT YET ASSIGNED

Relative stereochemistry.

● HCl ·

RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 2 OF 28 CAPLUS COPYRIGHT 2002 ACS
     2002:792123 CAPLUS
     137:294972
DN
     Preparation of substituted bicyclo[]-4-amino-pyridopyrimidine derivatives
     as kinase inhibitors
     Bhattacharya, Samit Kumar; Kath, John Charles; Morris, Joel
IN
     Pfizer Products Inc., USA
PA
SO
     Eur. Pat. Appl., 24 pp.
     CODEN: EPXXDW
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                     KIND DATE
                                          APPLICATION NO.
                           _____
                     ----
                                          ------
ΡI
     EP 1249451
                     A2
                           20021016
                                          EP 2002-252428
                                                          20020403
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
            IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
     JP 2002322178
                     A2
                           20021108
                                          JP 2002-102413
                                                          20020404
PRAI US 2001-283910P
                      Ρ
                           20010413
    MARPAT 137:294972
OS
GΙ
```

Title compds. I [R1-2 = H, alkyl; R3 = (CR1R2)mR4; m = 0-6 or NR1R3 = (CR1R2)n-indol(in)yl; n = 0-2; X = N and Y is CR9 or X = CR9 and Y = N; R9 = fused-ring bicyclic, bridged bicyclic or spirobicylic group] were prepd. For instance, 4-chloro-6-fluoropyrido[3,4-d]pyrimidine (prepn. given) was reacted with [3-methyl-4-(pyridin-3-yloxy)phenyl]amine (t-BuOH/ClCH2CH2Cl, reflux, 1 h) and the product coupled to (3-azabicyclo[3.1.0]hex-6-yl)carbamic acid tert-Bu ester (EtOH, sealed tube, 105.degree., 24 h) and finally deprotected to give II. Selected compds. of the invention had IC50 in the range of 1 nM to 1 pM for erbB-2 receptor kinase. I are used for the treatment of hyperproliferative disorders.

IT 468734-02-3P, [4-(2-Fluorophenoxy)-3-methylphenyl]-[6-

II

CN

(hexahydropyrrolo[3,4-c]pyrrol-2-yl)pyrido[3,4-d]pyrimidin-4-yl]amine RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of fused arylamino-substituted pyridopyrimidines as $\mbox{erb}B-2$ kinase inhibitors)

RN 468734-02-3 CAPLUS

```
ANSWER 3 OF 28 CAPLUS COPYRIGHT 2002 ACS
      2001:798225 CAPLUS
AN
      135:344471
DN
ΤI
      Preparation of diazabicyclic compounds as central nervous system active
      Schrimpf, Michael R.; Tietje, Karin R.; Toupence, Richard B.; Ji, Jianguo;
ΙN
      Basha, Anwer; Bunnelle, William H.; Daanen, Jerome F.; Pace, Jennifer M.;
      Sippy, Kevin B.
PA
      Abbott Laboratories, USA
      PCT Int. Appl., 190 pp.
      CODEN: PIXXD2
DT
      Patent
LΑ
      English
FAN.CNT 1
      PATENT NO.
                           KIND DATE
                                                    APPLICATION NO. DATE
                          ____
      WO 2001081347
                         - A2
                                  20011101
                                                    WO 2001-US13798 20010427
      WO 2001081347
                                  20020131
                          А3
               AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                CO, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM,
                HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS,
                LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO,
          RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
      US 2002019388
                                  20020214
                                                    US 2001-833914
                           A1
                                                                         20010412
      BR 2001007246
                                                    BR 2001-7246
                            Ά
                                  20021001
                                                                         20010427
PRAI US 2000-200111P
                                  20000427
      US 2000-559943 RBA
                                  20000427
      US 2001-833914
                                  20010412
      WO 2001-US13798
                            W
                                  20010427
os
     MARPAT 135:344471
GΙ
```

Diazabicyclic compds. (I; e.g. cis-2-(3-pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride), pharmaceutical compns. of these compds., and use of said compns. to control synaptic transmission in mammals are claimed. In I: A = covalent bond, CH2, CH2CH2, and CH2CH2CH2; B = CH2 and CH2CH2, provided that when A is CH2CH2CH2, then B is CH2; Y = covalent bond, CH2, and CH2CH2; Z = covalent bond, CH2, and CH2CH2, provided that when Y is CH2CH2, then Z is a covalent bond and further provided that when Z is CH2CH2, then Y is a covalent bond. R1 = optionally substituted phthalazin-1-yl, pyridin-3-yl, pyrazinyl, pyrimidin-5-yl, pyridazin-3-yl, quinolin-3-yl, thieno[3,2-b]pyridin-2-yl, furano[3,2-b]pyridin-2-yl, thieno[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-3-yl, furano[3,2-b]pyridin-3-yl,

6-yl, thieno[3,2-b]pyridin-6-yl, furano[2,3-b]pyridin-5-yl, thieno[2,3-b]pyridin-5-yl, isothiazol-5-yl, isoxazol-5-yl. R9 = H, alkoxycarbonyl, alkyl, amino, aminoalkyl, aminocarbonylalkyl, benzyloxycarbonyl, cyanoalkyl, dihydro-3-pyridinylcarbonyl, hydroxy, hydroxyalkyl, and phenoxycarbonyl. Values are reported for nicotinic acetylcholine receptor binding potencies and effectiveness of nicotinic acetylcholine receptor ligands as analgesic agents and in the formalin test for some of the claimed compds. Ninety-six example prepns. are given but the methods of prepn. are not claimed. The crystal and mol. structures of (3aS,6aS)-5-[(4-nitrophenyl)sulfonyl]-1-((1R)-1phenylethyl)octahydropyrrolo[3,4-b]pyrrole and tert-Bu (3S, 4S) - 4 - (hydroxymethyl) - 3 - [((1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - 1 - phenylethyl) amino] - 1 - (1S) - (1S)piperidinecarboxylate were detd. by x-ray crystallog. 370879-94-0P, cis-7-(6-Chloro-3-pyridinyl)-2,7diazabicyclo[3.3.0]octane RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (intermediate; prepn. of diazabicyclic compds. as central nervous system active agents) RN 370879-94-0 CAPLUS Pyrrolo[3,4-b]pyrrole, octahydro-5-(6-chloro-3-pyridinyl)-, (3aR,6aR)-rel-CN (9CI) (CA INDEX NAME)

Relative stereochemistry.

370879-59-7P, tert-Butyl cis-5-(3-pyridinyl)hexahydropyrrolo[3,4c]pyrrole-2(1H)-carboxylate 370879-64-4P, tert-Butyl cis-5-(6-chloro-3-pyridinyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)carboxylate 370879-66-6P, cis-2-(6-Chloro-3-pyridinyl)-5methyloctahydropyrrolo[3,4-c]pyrrole 370879-68-8P, tert-Butyl cis-5-(3-quinolinyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)-carboxylate 370879-70-2P, tert-Butyl cis-5-[5-(benzyloxy)-3pyridinyl]hexahydropyrrolo[3,4-c]pyrrole-2(1H)carboxylate 370879-71-3P, tert-Butyl cis-5-(5-hydroxy-3pyridinyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)-carboxylate 370879-73-5P, tert-Butyl cis-5-(5-methoxy-3pyridinyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)-carboxylate 370879-75-7P, tert-Butyl cis-5-(5-ethoxy-3pyridinyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)-carboxylate 370879-79-1P, tert-Butyl cis-5-(5-propoxy-3pyridinyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)-carboxylate 370879-81-5P, tert-Butyl cis-5-(6-chloro-5-methoxy-3pyridinyl)hexahydropyrrolo[3,4-c]pyrrole-2(1H)carboxylate **370879-83-7P**, tert-Butyl cis-5-(6-chloro-5-methyl 3-pyridinyl) hexahydropyrrolo[3,4-c]pyrrole-2(1H) carboxylate

```
370879-88-2P, tert-Butyl cis-5-[5-(2,2,2-trifluoroethoxy)-3-
pyridinyl]hexahydropyrrolo[3,4-c]pyrrole-2(1H)carboxylate
370879-90-6P, cis-1-Benzyl-5-(6-chloro-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370880-10-7P,
tert-Butyl (3aR,6aR)-5-(6-chloro-3-pyridinyl)hexahydropyrrolo[3,4-
b]pyrrole-1(2H)-carboxylate 370880-17-4P, tert-Butyl
(3aS, 6aS)-5-(6-chloro-3-pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)-
carboxylate 370880-33-4P, tert-Butyl cis-6-(6-chloro-3-
pyridinyl)octahydro-1H-pyrrolo[3,4-b]pyridine-1-carboxylate
370880-35-6P, tert-Butyl cis-6-(3-pyridinyl)octahydro-1H-
pyrrolo[3,4-b]pyridine-1-carboxylate 370880-37-8P, tert-Butyl
(3aR, 6aR) -5-(5, 6-dichloro-3-pyridinyl) hexahydropyrrolo[3, 4-b]pyrrole-
1(2H) carboxylate 370880-39-0P, tert-Butyl (3aS, 6aS)-5-(5, 6-
dichloro-3-pyridinyl) hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-41-4P, tert-Butyl (3aS,6aS)-5-(6-chloro-5-methyl-3-
pyridinyl) hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-43-6P, tert-Butyl (3aR, 6aR)-5-(6-chloro-5-methyl-3-
pyridinyl) hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-45-8P, tert-Butyl (3aR,6aR)-5-(3-
pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-47-0P, tert-Butyl (3aR,6aR)-5-(5-methoxy-3-
pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)carboxylate
370880-50-5P, tert-Butyl (3aS,6aS)-5-(3-
pyridinyl) hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-53-8P, tert-Butyl (3aS,6aS)-5-(5-bromo-3-
pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-56-1P, tert-Butyl (3aS, 6aS)-5-(5-methoxy-3-
pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)carboxylate
370880-65-2P, tert-Butyl (3aR, 6aR)-5-[5-[(trimethylsilyl)ethynyl]-
3-pyridinyl]hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-66-3P, tert-Butyl (3aR, 6aR)-5-(5-ethynyl-3-
pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-68-5P, tert-Butyl (3aR, 6aR)-5-(5-bromo-3-
pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370880-70-9P, tert-Butyl (3aR,6aR)-5-(5-cyano-3-
pyridinyl) hexahydropyrrolo[3,4-b]pyrrole-(2H)-carboxylate
370880-80-1P, tert-Butyl cis-3-(3-pyridinyl)-3,6-
diazabicyclo[3.2.0]heptane-6-carboxylate 370880-90-3P,
cis-3-(6-Chloro-3-pyridinyl)-3,6-diazabicyclo[3.2.0]heptane
370880-92-5P, tert-Butyl cis-3-(6-chloro-3-pyridinyl)-3,6-
diazabicyclo[3.2.0]heptane-6-carboxylate 370881-03-1P,
tert-Butyl (3aR, 6aR)-5-(6-bromo-5-methoxy-3-pyridinyl)hexahydropyrrolo[3,4-
b]pyrrole-1(2H)-carboxylate hydrochloride (4:7) 370881-31-5p,
tert-Butyl (3aR,6aR)-5-(6-bromo-5-cyano-3-pyridinyl)hexahydropyrrolo[3,4-
b]pyrrole-1(2H)-carboxylate 370881-77-9P, tert-Butyl
(3aR, 6aR) -5-(5-vinyl-3-pyridinyl) hexahydropyrrolo[3,4-b]pyrrole-1(2H)-
carboxylate 370881-78-0P, (3AR,6aR)-5-(5-vinyl-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370881-82-6P,
tert-Butyl (3aR,6aR)-5-(5-methyl-3-pyridinyl)hexahydropyrrolo[3,4-
b]pyrrole-1(2H)-carboxylate 370881-83-7P, (3AR,6aR)-5-(5-methyl-
3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370881-87-1P,
(3AR, 6aR) -5-(6-bromo-5-methyl-3-pyridinyl) octahydropyrrolo[3,4-b]pyrrole
370882-03-4P, tert-Butyl (3aR, 6aR)-5-(5-ethyl-3-
pyridinyl)hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370882-04-5P, [5-[(3AR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-
yl]-2-bromo-3-pyridinyl]methanol 370882-06-7P, tert-Butyl
(3aR, 6aR) -5-[5-(hydroxymethyl)-3-pyridinyl]hexahydropyrrolo[3,4-b]pyrrole-
1(2H)-carboxylate 370882-07-8P, tert-Butyl (3aR,6aR)-5-[6-bromo-
```

```
5-(hydroxymethyl)-3-pyridinyl]hexahydropyrrolo[3,4-b]pyrrole-1(2H)-
     carboxylate 370882-09-0P, tert-Butyl (3aR, 6aR)-5-(6-bromo-5-
     viny1-3-pyridiny1)hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
     370882-10-3P, (3AR, 6aR)-5-(6-bromo-5-vinyl-3-
     pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370882-11-4P,
     [5-[(3AR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-2-bromo-3-
     pyridinyl]acetonitrile 370882-13-6P, tert-Butyl
     (3aR, 6aR) -5-[6-bromo-5-[[(methylsulfonyl)oxy]methyl]-3-
     pyridinyl]hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
     370882-15-8P, (3AR, 6aR) -5-[6-bromo-5-(methoxymethyl)-3-
     pyridinyl]octahydropyrrolo[3,4-b]pyrrole 370882-17-0P,
     tert-Butyl (3aR, 6aR) -5-[6-bromo-5-(methoxymethyl)-3-
     pyridinyl]hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
     370882-62-5P, tert-Butyl (1S, 5R)-3-(5-cyano-3-pyridinyl)-3,6-
     diazabicyclo[3.2.0]heptane-6-carboxylate 370882-67-0P,
     tert-Butyl (1S,5R)-3-(6-chloro-3-pyridinyl)-3,6-diazabicyclo[3.2.0]heptane-
     6-carboxylate
     RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
     (Reactant or reagent)
        (intermediate; prepn. of diazabicyclic compds. as central nervous
        system active agents)
RN
     370879-59-7 CAPLUS
     Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(3-pyridinyl)-,
CN
     1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)
```

Relative stereochemistry.

RN 370879-64-4 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-66-6 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(6-chloro-3-pyridinyl)-5-methyl-,

(3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-68-8 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(3-quinolinyl)-, 1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-70-2 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-[5-(phenylmethoxy)-3-pyridinyl]-, 1,1-dimethylethyl ester, (3aR,6aS)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-71-3 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(5-hydroxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-73-5 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(5-methoxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-75-7 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, 5-(5-ethoxy-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-79-1 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(5-propoxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX

NAME)

Relative stereochemistry.

RN 370879-81-5 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(6-chloro-5-methoxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-83-7 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-(6-chloro-5-methyl-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aS)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-88-2 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-5-[5-(2,2,2-trifluoroethoxy)-3-pyridinyl]-, 1,1-dimethylethyl ester, (3aR,6aS)-rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-90-6 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-3-pyridinyl)octahydro-1-(phenylmethyl)-, (3aR,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370880-10-7 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(6-chloro-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-17-4 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(6-chloro-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX

NAME)

Absolute stereochemistry.

RN 370880-33-4 CAPLUS

CN 1H-Pyrrolo[3,4-b]pyridine-1-carboxylic acid, 6-(6-chloro-3-pyridinyl)octahydro-, 1,1-dimethylethyl ester, (4aR,7aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

514 - 300

RN 370880-35-6 CAPLUS

CN 1H-Pyrrolo[3,4-b]pyridine-1-carboxylic acid, octahydro-6-(3-pyridinyl)-, 1,1-dimethylethyl ester, (4aR,7aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370880-37-8 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5,6-dichloro-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-39-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5,6-dichloro-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-41-4 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(6-chloro-5-methyl-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-43-6 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(6-chloro-5-methyl-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-45-8 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, hexahydro-5-(3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-47-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, hexahydro-5-(5-methoxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-50-5 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, hexahydro-5-(3-pyridinyl)-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-53-8 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5-bromo-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-56-1 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, hexahydro-5-(5-methoxy-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-65-2 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, hexahydro-5-[5-[(trimethylsilyl)ethynyl]-3-pyridinyl]-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

MegSi
$$-C$$
 \subset C

 $t-BuO$
 N
 R
 N
 R

RN 370880-66-3 CAPLUS
CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5-ethynyl-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX

Absolute stereochemistry,

RN 370880-68-5 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5-bromo-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-70-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5-cyano-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-80-1 CAPLUS

CN 3,6-Diazabicyclo[3.2.0]heptane-6-carboxylic acid, 3-(3-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

514-338 546-276.7

RN 370880-90-3 CAPLUS

CN 3,6-Diazabicyclo[3.2.0]heptane, 3-(6-chloro-3-pyridinyl)- (9CI) (CA INDEX NAME)

RN 370880-92-5 CAPLUS

CN 3,6-Diazabicyclo[3.2.0]heptane-6-carboxylic acid, 3-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 370881-03-1 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(6-bromo-5-methoxy-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, hydrochloride (4:7),

(3aR, 6aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●7/4 HCl

RN 370881-31-5 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(6-bromo-5-cyano-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370881-77-9 CAPLUS

Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5-ethenyl-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370881-78-0 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5-ethenyl-3-pyridinyl)octahydro-, (3aR,6aR)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370881-82-6 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, hexahydro-6-(5-methyl-3-pyridinyl)-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370881-83-7 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(5-methyl-3-pyridinyl)-, (3aR,6aR)(9CI) (CA INDEX NAME)

09/833,914

Absolute stereochemistry.

RN 370881-87-1 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(6-bromo-5-methyl-3-pyridinyl)octahydro-, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-03-4 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(5-ethyl-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-04-5 CAPLUS

CN 3-Pyridinemethanol, 2-bromo-5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-06-7 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, hexahydro-5-[5-(hydroxymethyl)-3-pyridinyl]-, 1,1-dimethylethyl ester, (3aR,6aR)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-07-8 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-[6-bromo-5-(hydroxymethyl)-3-pyridinyl]hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-09-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-(6-bromo-5-ethenyl-3-pyridinyl)hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-10-3 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(6-bromo-5-ethenyl-3-pyridinyl)octahydro-, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-11-4 CAPLUS

CN 3-Pyridineacetonitrile, 2-bromo-5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-13-6 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-[6-bromo-5-[[(methylsulfonyl)oxy]methyl]-3-pyridinyl]hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-15-8 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-[6-bromo-5-(methoxymethyl)-3-pyridinyl]octahydro-, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-17-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-[6-bromo-5-(methoxymethyl)-

3-pyridinyl]hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-62-5 CAPLUS

CN 3,6-Diazabicyclo[3.2.0]heptane-6-carboxylic acid, 3-(5-cyano-3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-67-0 CAPLUS

CN 3,6-Diazabicyclo[3.2.0]heptane-6-carboxylic acid, 3-(6-chloro-3-pyridinyl)-, 1,1-dimethylethyl ester, (1S,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 370879-51-9P, cis-2-(3-Pyridinyl)octahydropyrrolo[3,4-c]pyrrole

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dihydrochloride 370879-61-1P, cis-2-Methyl-5-(3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride
370879-63-3P, cis-2-(6-Chloro-3-pyridinyl)octahydropyrrolo[3,4-
c]pyrrole monohydrochloride 370879-65-5P, cis-2-(6-Chloro-3-
pyridinyl)-5-methyloctahydropyrrolo[3,4-c]pyrrole dihydrochloride
370879-67-7P, cis-2-(3-Quinolinyl)octahydropyrrolo[3,4-c]pyrrole
dihydrochloride 370879-69-9P, cis-2-(5-Hydroxy-3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride
370879-72-4P, cis-2-(5-Methoxy-3-pyridinyl)octahydropyrrolo[3,4-
c]pyrrole dihydrochloride 370879-74-6P, cis-2-(5-Ethoxy-3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride
370879-76-8P, cis-2-(5-Propoxy-3-pyridinyl)octahydropyrrolo[3,4-
c]pyrrole 370879-77-9P, cis-2-(5-Propoxy-3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole semi(fumarate)
370879-80-4P, cis-2-(6-Chloro-5-methoxy-3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride
370879-82-6P, cis-2-(6-Chloro-5-methyl-3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole dihydrochloride
370879-85-9P, cis-2-[5-(2,2,2-Trifluoroethoxy)-3-
pyridinyl]octahydropyrrolo[3,4-c]pyrrole dihydrochloride
370879-89-3P, cis-5-(6-Chloro-3-pyridinyl)octahydropyrrolo[3,4-
b]pyrrole monohydrochloride 370879-96-2P, (3AR,6aR)-5-(6-chloro-
3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride
370880-11-8P, (3AS, 6aS)-5-(6-chloro-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride
370880-32-3P, cis-6-(6-Chloro-3-pyridinyl)octahydro-1H-pyrrolo[3,4-
b]pyridine dihydrochloride 370880-34-5P, cis-6-(3-
Pyridinyl)octahydro-1H-pyrrolo[3,4-b]pyridine dihydrochloride
370880-36-7P, (3AR, 6aR)-5-(5, 6-dichloro-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole monohydrochloride
370880-38-9P, (3AS, 6aS)-5-(5, 6-dichloro-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole monohydrochloride
370880-40-3P, (3AS, 6aS)-5-(6-chloro-5-methyl-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole hydrochloride (5:9)
370880-42-5P, (3AR, 6aR)-5-(6-chloro-5-methyl-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole hydrochloride (4:7)
370880-44-7P, (3AR, 6aR) -5-(3-pyridinyl) octahydropyrrolo[3, 4-
b]pyrrole dihydrochloride 370880-46-9P, (3AR, 6aR)-5-(5-methoxy-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride
370880-48-1P, (3AS, 6aS)-5-(3-pyridinyl)octahydropyrrolo[3,4-
b]pyrrole 370880-49-2P, (3AS, 6aS)-5-(3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole mono(4-methylbenzenesulfonate)
370880-51-6P, (3AS, 6aS)-5-(5-bromo-3-pyridinyl)octahydropyrrolo[3,
4-b]pyrrole 370880-52-7P, (3AS,6aS)-5-(5-bromo-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole mono(4-methylbenzenesulfonate)
370880-54-9P, (3AS, 6aS)-5-(5-methoxy-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370880-55-0P,
(3AS, 6aS)-5-(5-methoxy-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole
mono(4-methylbenzenesulfonate) 370880-64-1P,
(3AR, 6aR) -5 - (5 - ethynyl - 3 - pyridinyl) octahydropyrrolo [3, 4 - b] pyrrole
dihydrochloride 370880-67-4P, (3AR, 6aR)-5-(5-bromo-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride
370880-69-6P 370880-71-0P, 5-[(3AR,6aR)-
hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]nicotinonitrile monofumarate
370880-72-1P, cis-3-(3-Pyridinyl)-3,6-diazabicyclo[3.2.0]heptane
370880-73-2P, cis-3-(3-Pyridinyl)-3,6-diazabicyclo[3.2.0]heptane
bis(4-methylbenzenesulfonate) 370880-91-4P, cis-3-(6-Chloro-3-
pyridinyl)-3,6-diazabicyclo[3.2.0]heptane hemifumarate
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370881-02-0P, (3AR, 6aR)-5-(6-bromo-5-methoxy-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370881-29-1P,
5-[(3AR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-2-
bromonicotinonitrile 370881-30-4P, 5-[(3AR,6aR)-
hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-2-bromonicotinonitrile
monofumarate 370881-75-7P, (3AR, 6aR)-5-(5-vinyl-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride
370881-84-8P, (3AR, 6aR)-5-(6-bromo-5-chloro-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370881-85-9P,
(3AR, 6aR)-5-(6-bromo-5-chloro-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole
monofumarate 370881-86-0P, (3AR, 6aR)-5-(6-bromo-5-methyl-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride
370882-02-3P, (3AR, 6aR)-5-(5-ethyl-3-pyridinyl)octahydropyrrolo[3,
4-b]pyrrole 370882-05-6P, [5-[(3AR,6aR)-hexahydropyrrolo[3,4-
b]pyrrol-5(1H)-yl]-2-bromo-3-pyridinyl]methanol monofumarate
370882-08-9P, (3AR, 6aR)-5-(6-bromo-5-vinyl-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole dihydrochloride
370882-12-5P, [5-[(3AR, 6aR) -hexahydropyrrolo[3, 4-b]pyrrol-5(1H) -
yl]-2-bromo-3-pyridinyl]acetonitrile monofumarate 370882-14-7P,
tert-Butyl (3aR, 6aR) -5-[6-bromo-5-(cyanomethyl)-3-
pyridinyl]hexahydropyrrolo[3,4-b]pyrrole-1(2H)-carboxylate
370882-16-9P, (3AR, 6aR)-5-[6-bromo-5-(methoxymethyl)-3-
pyridinyl]octahydropyrrolo[3,4-b]pyrrole monofumarate 370882-60-3P
, 5-[(1R,5R)-3,6-Diazabicyclo[3.2.0]hept-3-yl]nicotinonitrile
370882-61-4P, 5-[(1R,5R)-3,6-Diazabicyclo[3.2.0]hept-3-
yl]nicotinonitrile monofumarate 370882-63-6P,
(1R,5R)-3-(6-Chloro-3-pyridinyl)-3,6-diazabicyclo[3.2.0]heptane
370882-64-7P, (1R,5R)-3-(6-Chloro-3-pyridinyl)-3,6-
diazabicyclo[3.2.0]heptane fumarate (10:11) 370883-36-6P,
(3AR, 6aR) -5-(6-chloro-3-pyridinyl) octahydropyrrolo[3,4-b]pyrrole
370883-37-7P, (3AS, 6aS)-5-(6-chloro-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370883-38-8P,
(3AR, 6aR) -5-(5, 6-dichloro-3-pyridinyl) octahydropyrrolo[3, 4-b]pyrrole
370883-39-9P, (3AS, 6aS)-5-(5, 6-dichloro-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370883-40-2P,
(3AS, 6aS)-5-(6-chloro-5-methyl-3-pyridinyl)octahydropyrrolo[3,4-b]pyrrole
370883-41-3P, (3AR,6aR)-5-(6-chloro-5-methyl-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370883-42-4P,
(3AR, 6aR) -5-(3-pyridinyl) octahydropyrrolo[3, 4-b]pyrrole
370883-43-5P, (3AR, 6aR) -5-(5-methoxy-3-
pyridinyl)octahydropyrrolo[3,4-b]pyrrole 370883-44-6P,
(3AR, 6aR) -5-(5-ethynyl-3-pyridinyl) octahydropyrrolo[3,4-b]pyrrole
370883-45-7P, (3AR, 6aR) -5-(5-bromo-3-pyridinyl) octahydropyrrolo[3,
4-b]pyrrole 370883-46-8P, 5-[(3AR,6aR)-hexahydropyrrolo[3,4-
b]pyrrol-5(1H)-yl]nicotinonitrile 370883-47-9P,
cis-2-(3-Pyridinyl)octahydropyrrolo[3,4-c]pyrrole 370883-48-0P,
cis-2-Methyl-5-(3-pyridinyl)octahydropyrrolo[3,4-c]pyrrole
370883-49-1P, cis-2-(6-Chloro-3-pyridinyl)octahydropyrrolo[3,4-
c]pyrrole 370883-50-4P, cis-2-(3-Quinolinyl)octahydropyrrolo[3,4-
c]pyrrole 370883-52-6P, cis-2-(5-Hydroxy-3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole 370883-54-8P,
cis-2-(5-Methoxy-3-pyridinyl)octahydropyrrolo[3,4-c]pyrrole
370883-56-0P, cis-2-(5-Ethoxy-3-pyridinyl)octahydropyrrolo[3,4-
c]pyrrole 370883-59-3P, cis-2-(6-Chloro-5-methoxy-3-
pyridinyl)octahydropyrrolo[3,4-c]pyrrole 370883-60-6P,
cis-2-(6-Chloro-5-methyl-3-pyridinyl)octahydropyrrolo[3,4-c]pyrrole
370883-61-7P, cis-2-[5-(2,2,2-Trifluoroethoxy)-3-
pyridinyl]octahydropyrrolo[3,4-c]pyrrole 370883-62-8P,
```

Relative stereochemistry.

●2 HCl

RN 370879-61-1 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, octahydro-2-methyl-5-(3-pyridinyl)-,
dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HC1

RN 370879-63-3 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, 2-(6-chloro-3-pyridinyl)octahydro-,
monohydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 370879-65-5 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(6-chloro-3-pyridinyl)-5-methyl-, dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

RN 370879-67-7 CAPLUS

CN Quinoline, 3-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-, dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

09/833,914

RN 370879-69-9 CAPLUS

CN 3-Pyridinol, 5-[(3aR,6aS)-hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl]-, dihydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HC1

RN 370879-72-4 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(5-methoxy-3-pyridinyl)-, dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

RN 370879-74-6 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(5-ethoxy-3-pyridinyl)octahydro-, dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

•2 HCl

RN 370879-76-8 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(5-propoxy-3-pyridinyl)-,
(3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370879-77-9 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(5-propoxy-3-pyridinyl)-,
(3aR,6aS)-rel-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370879-76-8 CMF C14 H21 N3 O

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

$$_{\rm HO_2C}$$
 $^{\rm E}$ $_{\rm CO_2H}$

RN 370879-80-4 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(6-chloro-5-methoxy-3-pyridinyl)-, dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

•2 HCl

RN 370879-82-6 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(6-chloro-5-methyl-3-pyridinyl)-, dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

•2 HCl

RN 370879-85-9 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, octahydro-2-[5-(2,2,2-trifluoroethoxy)-3-pyridinyl], dihydrochloride, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

RN 370879-89-3 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(6-chloro-3-pyridinyl)-,
monohydrochloride, (3aR,6aR)-rel- (9CI) (CA INDEX NAME)

RN 370879-96-2 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(6-chloro-3-pyridinyl)-, dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HCl

RN 370880-11-8 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-3-pyridinyl)octahydro-,
dihydrochloride, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HC1

09/833,914

RN 370880-32-3 CAPLUS

CN 1H-Pyrrolo[3,4-b]pyridine, 6-(6-chloro-3-pyridinyl)octahydro-, dihydrochloride, (4aR,7aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

RN 370880-34-5 CAPLUS

CN 1H-Pyrrolo[3,4-b]pyridine, octahydro-6-(3-pyridinyl)-, dihydrochloride, (4aR,7aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

RN 370880-36-7 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(5,6-dichloro-3-pyridinyl)octahydro-, monohydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

RN 370880-38-9 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5,6-dichloro-3-pyridinyl)octahydro-,
monohydrochloride, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 370880-40-3 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-5-methyl-3-pyridinyl)octahydro-,
hydrochloride (5:9), (3aS,6aS)- (9CI) (CA INDEX NAME)

●9/5 HCl

RN 370880-42-5 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-5-methyl-3-pyridinyl)octahydro-,
hydrochloride (4:7), (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●7/4 HCl

RN 370880-44-7 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(3-pyridinyl)-, dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

RN 370880-46-9 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(5-methoxy-3-pyridinyl)-,
dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HCl

RN 370880-48-1 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(3-pyridinyl)-, (3aS,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-49-2 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(3-pyridinyl)-, (3aS,6aS)-,

mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 370880-48-1 CMF C11 H15 N3

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 370880-51-6 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5-bromo-3-pyridinyl)octahydro-, (3aS,6aS)- (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

RN 370880-52-7 CAPLUS

Pyrrolo[3,4-b]pyrrole, 5-(5-bromo-3-pyridinyl)octahydro-, (3aS,6aS)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

09/833,914

CRN 370880-51-6 CMF C11 H14 Br N3

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 370880-54-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(5-methoxy-3-pyridinyl)-, (3aS,6aS)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370880-55-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(5-methoxy-3-pyridinyl)-, (3aS,6aS)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

09/833,914

CRN 370880-54-9 CMF C12 H17 N3 O

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 370880-64-1 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(5-ethynyl-3-pyridinyl)octahydro-, dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HCl

RN 370880-67-4 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(5-bromo-3-pyridinyl)octahydro-, dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HC1

RN 370880-69-6 CAPLUS

N 3-Pyridinecarbonitrile, 5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370880-71-0 CAPLUS

CN 3-Pyridinecarbonitrile, 5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-, rel-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370880-69-6 CMF C12 H14 N4

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 370880-72-1 CAPLUS

CN 3,6-Diazabicyclo[3.2.0]heptane, 3-(3-pyridinyl)- (9CI) (CA INDEX NAME)

RN 370880-73-2 CAPLUS

CN 3,6-Diazabicyclo[3.2.0]heptane, 3-(3-pyridinyl)-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 370880-72-1 CMF C10 H13 N3

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 370880-91-4 CAPLUS CN 3,6-Diazabicyclo[3.2.0]heptane, 3-(6-chloro-3-pyridinyl)-, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370880-90-3 CMF C10 H12 C1 N3

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 370881-02-0 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-bromo-5-methoxy-3-pyridinyl)octahydro-,
(3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370881-29-1 CAPLUS
CN 3-Pyridinecarbonitrile, 2-bromo-5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370881-30-4 CAPLUS

CN 3-Pyridinecarbonitrile, 2-bromo-5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-29-1 CMF C12 H13 Br N4

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 370881-75-7 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(5-ethenyl-3-pyridinyl)octahydro-, dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

RN 370881-84-8 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-bromo-5-chloro-3-pyridinyl)octahydro-,
(3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370881-85-9 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-bromo-5-chloro-3-pyridinyl)octahydro-,
(3aR,6aR)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370881-84-8 CMF C11 H13 Br C1 N3

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 370881-86-0 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(6-bromo-5-methyl-3-pyridinyl)octahydro-, dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

●2 HCl

RN 370882-02-3 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5-ethyl-3-pyridinyl)octahydro-, (3aR,6aR)- (9CI)
(CA INDEX NAME)

RN 370882-05-6 CAPLUS

CN 3-Pyridinemethanol, 2-bromo-5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-, (2E)-2-butenedioate (1:1) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-04-5 CMF C12 H16 Br N3 O

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 370882-08-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(6-bromo-5-ethenyl-3-pyridinyl)octahydro-, dihydrochloride, (3aR,6aR)- (9CI) (CA INDEX NAME)

•2 HCl

RN 370882-12-5 CAPLUS

CN 3-Pyridineacetonitrile, 2-bromo-5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-11-4 CMF C13 H15 Br N4

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

$$HO_2C$$
 E CO_2H

RN 370882-14-7 CAPLUS
CN Pyrrolo[3,4-b]pyrrole-1(2H)-carboxylic acid, 5-[6-bromo-5-(cyanomethyl)-3-

pyridinyl]hexahydro-, 1,1-dimethylethyl ester, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-16-9 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-[6-bromo-5-(methoxymethyl)-3-pyridinyl]octahydfo-, (3aR,6aR)-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-15-8 CMF C13 H18 Br N3 O

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 370882-60-3 CAPLUS
CN 3-Pyridinecarbonitrile, 5-(1R,5R)-3,6-diazabicyclo[3.2.0]hept-3-yl- (9CI)

(CA INDEX NAME)

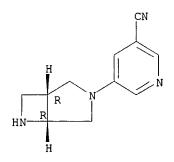
Absolute stereochemistry.

RN 370882-61-4 CAPLUS CN 3-Pyridinecarbonitrile, 5-(1R,5R)-3,6-diazabicyclo[3.2.0]hept-3-yl-, (2E)-2-butenedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-60-3 CMF C11 H12 N4

Absolute stereochemistry.



CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

RN 370882-63-6 CAPLUS CN 3,6-Diazabicyclo[3.2.0]heptane, 3-(6-chloro-3-pyridinyl)-, (1R,5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370882-64-7 CAPLUS
CN 3,6-Diazabicyclo[3.2.0]heptane, 3-(6-chloro-3-pyridinyl)-, (1R,5R)-, (2E)-2-butenedioate (10:11) (9CI) (CA INDEX NAME)

CM 1

CRN 370882-63-6 CMF C10 H12 C1 N3

Absolute stereochemistry.

CM 2

CRN 110-17-8 CMF C4 H4 O4

Double bond geometry as shown.

$$HO_2C$$
 E CO_2H

RN 370883-36-6 CAPLUS

CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-3-pyridinyl)octahydro-, (3aR,6aR)- (9CI) (CA INDEX NAME)

RN 370883-37-7 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-3-pyridinyl)octahydro-, (3aS,6aS)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-38-8 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5,6-dichloro-3-pyridinyl)octahydro-, (3aR,6aR)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-39-9 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5,6-dichloro-3-pyridinyl)octahydro-, (3aS,6aS)(9CI) (CA INDEX NAME)

RN 370883-40-2 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-5-methyl-3-pyridinyl)octahydro-,
(3as,6as)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-41-3 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(6-chloro-5-methyl-3-pyridinyl)octahydro-,
(3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-42-4 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(3-pyridinyl)-, (3aR,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-43-5 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, octahydro-5-(5-methoxy-3-pyridinyl)-, (3aR,6aR)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-44-6 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5-ethynyl-3-pyridinyl)octahydro-, (3aR,6aR)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-45-7 CAPLUS
CN Pyrrolo[3,4-b]pyrrole, 5-(5-bromo-3-pyridinyl)octahydro-, (3aR,6aR)- (9CI)
(CA INDEX NAME)

RN 370883-46-8 CAPLUS

CN 3-Pyridinecarbonitrile, 5-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 370883-47-9 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(3-pyridinyl)-, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370883-48-0 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-methyl-5-(3-pyridinyl)-, (3aR,6aS)-rel-(9CI) (CA INDEX NAME)

RN 370883-49-1 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, 2-(6-chloro-3-pyridinyl)octahydro-, (3aR,6aS)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370883-50-4 CAPLUS
CN Quinoline, 3-[(3aR,6aS)-hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl]-, rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370883-52-6 CAPLUS
CN 3-Pyridinol, 5-[(3aR,6aS)-hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl]-, rel(9CI) (CA INDEX NAME)

RN 370883-54-8 CAPLUS CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(5-methoxy-3-pyridinyl)-, (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370883-56-0 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(5-ethoxy-3-pyridinyl)-, (3aR,6aS)-rel(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370883-59-3 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, 2-(6-chloro-5-methoxy-3-pyridinyl)octahydro-,
(3aR,6aS)-rel- (9CI) (CA INDEX NAME)

RN 370883-60-6 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, 2-(6-chloro-5-methyl-3-pyridinyl)octahydro-,
(3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370883-61-7 CAPLUS
CN Pyrrolo[3,4-c]pyrrole, octahydro-2-[5-(2,2,2-trifluoroethoxy)-3-pyridinyl], (3aR,6aS)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 370883-63-9 CAPLUS CN 1H-Pyrrolo[3,4-b]pyridine, octahydro-6-(3-pyridinyl)-, (4aR,7aR)-rel-(9CI) (CA INDEX NAME)

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ANSWER 4 OF 28 CAPLUS COPYRIGHT 2002 ACS
    2001:573269 CAPLUS
     135:152805
DN
     Preparation of benzimidazoles as ORL1-receptor agonists for analgesics
ΤI
    Ito, Fumitaka; Noguchi, Hirohide; Ohashi, Yoriko; Shimokawa, Hirohisa
IN
     Pfizer Pharmaceutical Co., Ltd., Japan
     Jpn. Kokai Tokkyo Koho, 39 pp.
     CODEN: JKXXAF
DΤ
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    PATENT NO.
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PRAI US 2000-174542P

MARPAT 135:152805

AB Title compds. I [R1 = C3-11 cycloalkyl, C6-16 bicycloalkyl, C6-16 tricycloalkyl, C8-16 tetracycloalkyl, etc.; A = (un)substituted C1-7 alkyl, C2-5 alkenyl, C2-5 alkynyl, aryl, etc.; M = single bond, CH2,O, S, SO, SO2, CO, NH, etc.; Y = 4- to 12-membered bicyclic carbon ring, 4- to 12-membered bicyclic hetero ring, 5- to 17-membered spiro carbon ring, 5- to 17-membered spiro hetero ring; Z1-Z4 = (un)substituted C1-4 alkyl, C1-4 alkoxy, C1-4 alkylsulfonyl, C1-4 alkylcarbonyl, carboxy, etc.] or their salts are prepd. Tert-Bu 3-[1-(1-(1-phenylcycloheptyl)-4-piperidinyl]-1H-benzimidazol-2-yl]-3,8-diazabicyclo[3.2.1]octane-8-carboxylate was treated with F3CCO2H in CH2Cl2 at room temp. for 0.5 h to give 77.6% 2-(3,8-diazabicyclo[3.2.1]oct-3-yl)-1-[1-(1-phenylcycloheptyl)-4-piperidinyl]-1H-benzimidazole HCl salt.

IT 352542-61-1DP, mesylate

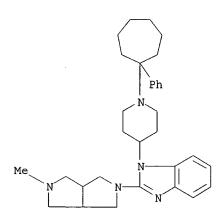
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of benzimidazoles as ORL1-receptor agonists for analgesics)

RN 352542-61-1 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-2(1H)-carboxylic acid, hexahydro-1-(hydroxymethyl)-5-[1-[1-(1-methylcyclooctyl)-4-piperidinyl]-1H-benzimidazol-2-yl]-, 1,1-dimethylethyl ester, (1R,3aS,6aR)-rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 352542-11-1 CAPLUS
CN 1H-Benzimidazole, 2-(hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)-1-[1-(1-phenylcycloheptyl)-4-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 352542-20-2 CAPLUS
CN 1H-Benzimidazole, 2-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

RN 352542-21-3 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 352542-22-4 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

RN 352542-23-5 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 352542-24-6 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

RN 352542-25-7 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

RN 352542-38-2 CAPLUS

CN 1H-Benzimidazole, 1-[1-(1-methylcyclooctyl)-4-piperidinyl]-2-(octahydro-2H-pyrrolo[3,4-c]pyridin-2-yl)- (9CI) (CA INDEX NAME)

RN 352542-39-3 CAPLUS

CN 1H-Benzimidazole, 1-[1-(1-methylcyclooctyl)-4-piperidinyl]-2-(octahydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

09/833,914

● HCl

RN 352542-40-6 CAPLUS

CN 1H-Benzimidazole, 1-[1-(1-methylcyclooctyl)-4-piperidinyl]-2-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)- (9CI) (CA INDEX NAME)

RN 352542-41-7 CAPLUS

CN 1H-Benzimidazole, 1-[1-(1-methylcyclooctyl)-4-piperidinyl]-2-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 352542-50-8 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydro-2-methylpyrrolo[3,4-b]pyrrol-5(1H)-yl)-1-[1-

Page 69

(1-methylcyclooctyl)-4-piperidinyl]- (9CI) (CA INDEX NAME)

RN 352542-51-9 CAPLUS

CN 1H-Benzimidazole, 2-(hexahydro-2-methylpyrrolo[3,4-b]pyrrol-5(1H)-yl)-1-[1-(1-methylcyclooctyl)-4-piperidinyl]-, monohydrochloride (9CI) (CA INDEX NAME)

HC1

```
ANSWER 5 OF 28 CAPLUS COPYRIGHT 2002 ACS
     2001:545673 CAPLUS
     135:122511
     Preparation of 3-aminoquinazoline-2,4-dione antibacterial agents
     Bird, Paul; Ellsworth, Edmund Lee; Nguyen, Dai Quoc; Sanchez, Joseph
     Peter; Showalter, Howard Daniel Hollis; Singh, Rajeshwar; Stier, Michael
     Andrew; Tran, Tuan Phong; Watson, Brian Morgan; Yip, Judy
     Warner-Lambert Company, USA
PΑ
     PCT Int. Appl., 291 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                                                APPLICATION NO. DATE
                         KIND DATE
                        ____
                               _____
     WO 2001053273
                         A1
                               20010726
                                                WO 2000-US33656 20001212
             AE, AG, AL, AU, BA, BB, BG, BR, BZ, CA, CN, CR, CU, CZ, DM, DZ,
              EE, GD, GE, HR, HU, ID, IL, IN, IS, JP, KP, KR, LC, LK, LR, LT,
              LV, MA, MG, MK, MN, MX, MZ, NO, NZ, PL, RO, SG, SI, SK, SL, TR,
              TT, UA, US, UZ, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
          RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     EP 1255739
                         A1
                               20021113
                                                EP 2000-984246 20001212
          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR
PRAI US 2000-178252P
                                20000124
                        P
     US 2000-241267P
                         Ρ
                                20001018
     WO 2000-US33656
                                20001212
                         W
     MARPAT 135:122511
GΙ
```

AB Title compds. (I) [wherein: R1 and R3 = independently H or (un)substituted (cyclo)alkyl, alkenyl, alkynyl, (hetero)aryl, or heterocyclic; independently R5, R6, and R8 = H or (un)substituted alkyl, alkenyl, alkynyl, or halo, NO2, CN, NH2, (di)alkylamino, etc.; or R1 and R8 taken together with the atoms to which they are attached may form an (un)substituted heterocycle; R7 = H or (un)substituted alkyl, alkenyl, alkynyl, (fused) heterocyclic, or (fused) aryl, or halo, NO2, CN, NH2, (di)alkylamino, carboxy, etc.; J and K = independently C or N; and pharmaceutically acceptable salts thereof] were prepd. as antibacterial agents. For example, N'-{4-[3-(tert-butoxycarbonylaminomethyl)pyrrolidin-1-yl]-2-cyclopropylamino-5-fluorobenzoyl)hydrazinecarboxylic acid tert-Bu

ester (multi-step prepn. given) was chlorinated with N-chlorosuccinimide, cyclized with triphosgene in the presence of K2CO3, and deprotected using HCl gas to afford II.bul.HCl. In antibacterial assays, II.bul.HCl exhibited min. inhibitory concns. of 0.13-2.0 .mu.g/mL against an assortment of Gram neg. and Gram pos. organisms, as well as ciprofloxacin resistant E. coli and S. aureus strains. In addn., II.bul.HCl inhibited supercoiling activity of DNA gyrase with IC50 of 1.0 .mu.M.

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(comparison compd.; prepn. of 3-aminoquinazoline-2,4-dione antibacterial agents via multi-step syntheses involving cyclization of benzoylhydrazinecarboxylates with phosgene)

RN 224189-78-0 CAPLUS

2,4(1H,3H)-Quinazolinedione, 1-cyclopropyl-6-fluoro-3-hydroxy-7-[(4aR,7aR)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

IT 351360-24-2P 351366-14-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; prepn. of 3-aminoquinazoline-2,4-dione antibacterial agents via multi-step syntheses involving cyclization of benzoylhydrazinecarboxylates with phosgene)

RN 351360-24-2 CAPLUS

Carbamic acid, [8-chloro-1-cyclopropyl-6-fluoro-7-(hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)-1,4-dihydro-2,4-dioxo-3(2H)-quinazolinyl]-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

RN 351366-14-8 CAPLUS

CN 1H-Pyrrolo[3,4-b]pyridine-1-carboxylic acid, 6-(3-amino-1-cyclopropyl-6-

CN

fluoro-1,2,3,4-tetrahydro-8-methyl-2,4-dioxo-7-quinazolinyl)octahydro-,
. 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 351362-69-1P 351363-48-9P 351366-04-6P 351371-78-3P 351372-02-6P 351372-52-6P 351372-83-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of 3-aminoquinazoline-2,4-dione antibacterial agents via multi-step syntheses involving cyclization of benzoylhydrazinecarboxylates with phosgene)

RN 351362-69-1 CAPLUS

CN Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 3-amino-1-cyclopropyl-6-fluoro-7-[(3as,7as)-octahydro-2H-pyrrolo[3,4-c]pyridin-2-yl]-, hydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

•x HCl

RN 351363-48-9 CAPLUS CN 2,4(1H,3H)-Quinazol:

2,4(1H,3H)-Quinazolinedione, 3-amino-8-chloro-1-cyclopropyl-6-fluoro-7-(hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)-, hydrochloride (9CI) (CA INDEX NAME)

RN 351366-04-6 CAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-amino-1-cyclopropyl-6-fluoro-8-methyl-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-, hydrochloride (9CI) (CA INDEX NAME)

●x HCl

RN 351371-78-3 CAPLUS

N Pyrido[2,3-d]pyrimidine-2,4(1H,3H)-dione, 3-amino-1-cyclopropyl-6-fluoro-7-(octahydro-2H-pyrrolo[3,4-c]pyridin-2-yl)- (9CI) (CA INDEX NAME)

RN 351372-02-6 CAPLUS

2,4(1H,3H)-Quinazolinedione, 3-amino-8-chloro-1-cyclopropyl-6-fluoro-7-(hexahydro-5-methylpyrrolo[3,4-c]pyrrol-2(1H)-yl)- (9CI) (CA INDEX NAME)

RN 351372-52-6 CAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-amino-1-cyclopropyl-6-fluoro-8-methyl-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
H & Me \\
N & N \\
\hline
N & NH_2
\end{array}$$

RN 351372-83-3 CAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 3-amino-1-cyclopropyl-6-fluoro-8-methoxy-7-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RE.CNT 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
L18 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2002 ACS
      2001:453062 CAPLUS
AN
DN
      135:61360
      Preparation of heteroaryldiazabicycloalkanes as nicotinic cholinergic
      receptor ligands.
IN
      Peters, Dan; Olsen, Gunnar M.; Nielsen, Elsebet Ostergaard; Nielsen, Simon
      Feldbaek; Ahring, Philip K.; Jorgensen, Tino Dyhring
PΑ
      Neurosearch A/S, Den.
      PCT Int. Appl., 34 pp.
      CODEN: PIXXD2
DT
      Patent
     English
LΑ
FAN. CNT 1
      PATENT NO.
                           KIND DATE
                                                      APPLICATION NO.
                                                                           DATE
                                                      _____
      WO 2001044243
                            A2
                                   20010621
                                                      WO 2000-DK696
                                                                           20001214
      WO 2001044243
                            A3
                                   20021031
           W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
                CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR,
                HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT,
          LU, LV, MA, MD, MG, MK, MN, MW, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM

RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
                BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
PRAI DK 1999-1790
                                   19991214
                            Α
      MARPAT 135:61360
GI
```



Ι

AB Title compds. [I; Z = (CH2)n; n = 0-2; R = H, alkyl, aryl, aralkyl, fluorescent group; R1 = (substituted) mono- or polyheterocyclyl], were prepd. as drugs and diagnostic agents (no data). Thus, 3,7-dibenzyl-3,7-diazabicyclo[3.3.1]nonane (prepn. given) was stirred with HCO2H and Pd/C to give crude monobenzyl deriv., which was heated with 2-chloroquinoline at 100.degree. for 1 h to give 7-benzyl-3-(2-quinolinyl)-3,7-diazabicyclo[3.3.1]nonane. I may be useful for the treatment of central nervous system diseases, disorders related to smooth muscle contraction, endocrine diseases or disorders, diseases or disorders related to neurodegeneration inflammation, pain, and drug withdrawal symptoms.

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IT 345316-85-0P 345316-88-3P 345316-90-7P
345316-96-3P 345316-97-4P 345316-99-6P
345317-01-3P 345317-03-5P 345317-05-7P
345317-06-8P 345317-07-9P 345317-08-0P
345317-09-1P 345317-10-4P 345317-11-5P
345317-12-6P 345317-13-7P 345317-14-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
```

BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of heteroaryldiazabicycloalkanes as nicotinic cholinergic receptor ligands)

RN 345316-85-0 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(3-pyridinyl)- (9CI) (CA INDEX NAME)

RN 345316-88-3 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(5-ethoxy-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345316-90-7 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(5-phenyl-3-pyridinyl)- (9CI) (CA INDEX NAME)

RN 345316-96-3 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-[5-(1H-pyrrol-1-yl)-3-pyridinyl]- (9CI) (CA INDEX NAME)

RN 345316-97-4 CAPLUS

CN 1H-Indole, 1-[5-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-y1)-3-pyridinyl]-(9CI) (CA INDEX NAME)

RN 345316-99-6 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(5-chloro-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345317-01-3 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(5-bromo-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345317-03-5 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(5-fluoro-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345317-05-7 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(5-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)

RN 345317-06-8 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-[6-(ethylthio)-3-pyridinyl]octahydro- (9CI) (CA INDEX NAME)

RN 345317-07-9 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-[5-(ethylthio)-3-pyridinyl]octahydro- (9CI) (CA INDEX NAME)

RN 345317-08-0 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-[5-(trifluoromethyl)-3-pyridinyl]-(9CI) (CA INDEX NAME)

RN 345317-09-1 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(6-fluoro-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345317-10-4 CAPLUS

Page 79

CN Pyrrolo[3,4-c]pyrrole, 2-(6-chloro-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345317-11-5 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(6-bromo-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345317-12-6 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(6-iodo-3-pyridinyl)- (9CI) (CA INDEX NAME)

RN 345317-13-7 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(5-ethyl-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

RN 345317-14-8 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2-(5-ethynyl-3-pyridinyl)octahydro- (9CI) (CA INDEX NAME)

8 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2002 ACS

2001:120739 CAPLUS

DN 134:326572

TI Chiral bicyclic phosphoramidites - a new class of ligands for asymmetric catalysis

AU Huttenloch, Oliver; Spieler, Jan; Waldmann, Herbert

CS Max-Planck-Institut fur molekulare Physiologie Abteilung Chemische Biologie, Dortmund, 44227, Germany

SO Chemistry—A European Journal (2001), 7(3), 671-675 CODEN: CEUJED; ISSN: 0947-6539

PB Wiley-VCH Verlag GmbH

DT Journal

LA English

OS CASREACT 134:326572

AB The development of new ligands for catalytic asym. C-C bond formation is of great interest to org. synthesis. The prepn. of new class of chiral phosphoramidites that embody one or two binaphthol units attached to an achiral azabicyclic [3.3.1] or [3.3.0] framework is described. These ligands were easily accessible from (R)-1,1'-binaphthyl-2,2'-dioxaphosphor-chloridite and the corresponding heterobicyclic core. They were employed in enantioselective Cu-catalyzed addns. of different dialkylzinc reagents to cyclic and acyclic enones. The chiral ketones were obtained with an enantiomeric ratio up to 91:9. The choice of the best ligand proved to be strongly dependent on each substrate. In addn., ligand derived from 1,5-dimethyl-3,7-diazabicyclo[3.3.0]octane was the most suitable for Rh-catalyzed hydrogenations of .alpha.,.beta.-unsatd. esters, giving rise to di-Me 2-methylsuccinate and Me N-acetylalaninate with enantiomer ratios up to 95:5.

IT 335616-65-4P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(prepn. of chiral bicyclic phosphoramidites as new class of ligands for asym. catalysis)

RN 335616-65-4 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, 2,5-bis[(11bR)-dinaphtho[2,1-d:1',2'-f][1,3,2]dioxaphosphepin-4-yl]octahydro-3a,6a-dimethyl-, cis-(9CI) (CFINDEX NAME)

RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 8 OF 28 CAPLUS COPYRIGHT 2002 ACS
     2000:666717 CAPLUS
ΑN
     133:252420
DN
     Preparation of heterocyclylmethylene oxazolones as selective
     .alpha.1-adrenoreceptor antagonists
     Coffen, David Llewellyn; Dillon, Michael Patrick; Ford, Anthony P. D. W.;
IN
     Gogas, Kathleen Ruth; Jacobson, Lupita; Li, Zhe; Williams, Timothy James
PA
     F. Hoffmann-La Roche A.-G., Switz.
SO
     PCT Int. Appl., 130 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
                      KIND DATE
                                             APPLICATION NO. DATE
     PATENT NO.
     ______
                                              ______
                                             WO 2000-EP2200 20000313
     WO 2000055143
                       A1 20000921
PΙ
         W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ,
              DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS,
              JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG,
              MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ,
              MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
     US 6355641
                        B1 20020312
                                              US 2000-521185 20000308
PRAI US 1999-124721P
                       P
                              19990317
     US 1999-124781P
                       P
                              19990317
     US 1999-165312P P
                              19991112
     MARPAT 133:252420
GΙ
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$$A = -N$$

$$A = -N$$

$$C = -N$$

$$R^{1} I$$

$$C = -N$$

$$R^{2} R^{2} R^{2}$$

$$R^{2} R^{2}$$

The title compds. (I) [wherein X = Formula (A), (B) or (C); m = 1-6; n = 1-60-5; p and q = independently 1-3 with the proviso that when p > 1, q = 1; Y = (CH2) wR3, (CH2) wCOR4, (CH2) wCONHR5, (CH2) wC(NR6) NHR7, (CH2) wSO2R8, (CH2) wNHR9, (CH2) wNHCOR10, (CH2) wNHCONHR11, or (CH2) wNHSO2R12; w = 0-3; Z = CH or N; R1 = cycloalkyl, cycloalkenyl, heterocyclic, or (hetero)aryl; R2a, R2b, and R2c = independently H, (cyclo)alkyl, alkenyl, or aryl(alkyl); or R2a and R2b form a 5- to 7-membered ring with the carbons to which they are attached; R3 = heterocyclic or heteroaryl; R4, R5, R8, R9, R10, R11, and R12 = independently H, (hydroxy)alkyl, alkoxy, alkylthio, alkenyl, cycloalkyl(alkyl), cycloalkenyl(alkyl), heterocyclic(alkyl), aryl(alkyl), or heteroaryl(alkyl); R6 and R7 = independently H, (hydroxy)alkyl, alkenyl, cycloalkyl(alkyl), cycloalkenyl(alkyl), heterocylic(alkyl), aryl(alkyl) or heteroaryl(alkyl)] where prepd. as selective .alpha.1-adrenoreceptor modulators, particularly antagonists. Thus, alkylation of N-phenylpiperazine-1-carboxamidine (prepn. given) with 4-ethoxymethylene-2-naphthalen-1-yl-4H-oxazol-5-one in DMSO gave II. In assays on the pain response to radiant heat and cold allodynia response in neuropathic rats, II had a significant effect at doses ranging from 30 .mu.g/kg to 1000 .mu.g/kg. I were tested in a [3H]prazosin binding assay and found to be selective .alpha.1Badrenoceptor antagonists. I are useful in the treatment of disorders of the urinary tract, including obstruction of the urinary tract, sexual dysfunction, pain, hypertension, and cardiac dysfunction. Examples of representative pharmaceutical formulations contg. I are also included.

IT 295340-63-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of heterocyclylmethylene oxazolones as selective .alpha.1B-adrenoreceptor antagonists by alkylation of ethoxymethylene

09/833,914

oxazolones with heterocycles)

RN 295340-63-5 CAPLUS

CN 5(4H)-Oxazolone, 4-[[5-(1H-benzimidazol-2-yl)hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl]methylene]-2-(4-benzofuranyl)- (9CI) (CA INDEX NAME)

IT 295341-57-0P, 2-(Hexahydropyrrolo[3,4-c]pyrrol-2-yl)-1H-

benzimidazole hydrochloride 295341-58-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of heterocyclylmethylene oxazolones as selective

.alpha.lB-adrenoreceptor antagonists by alkylation of ethoxymethylene oxazolones with heterocycles) $\,$

RN 295341-57-0 CAPLUS

● HCl

RN 295341-58-1 CAPLUS

CN 1H-Benzimidazole, 2-[hexahydro-5-(phenylmethyl)pyrrolo[3,4-h]pyrrol-2(1H)-yl]- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 9 OF 28 CAPLUS COPYRIGHT 2002 ACS

1999:572661 CAPLUS

131:351212

TI Synthesis and antimicrobial activity of 4H-4-oxoquinolizine derivatives: consequences of structural modification at the C-8 position

AU Ma, Zhenkun; Chu, Daniel T. W.; Cooper, Curt S.; Li, Qun; Fung, Anthony K. L.; Wang, Sanyi; Shen, Linus L.; Flamm, Robert K.; Nilius, Angela M.; Alder, Jeffery D.; Meulbroek, Jonathan A.; Or, Yat Sun

CS Infectious Disease Research, Abbott Laboratories, Abbott Park, IL, 60064-3537, USA

SO Journal of Medicinal Chemistry (1999), 42(20), 4202-4213 CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

GΙ

The antibacterial 4H-4-oxoquinolizines were introduced recently to overcome bacterial resistance to fluoroquinolones. They exhibit potent antibacterial activity against Gram-pos., Gram-neg., and anaerobic organisms and are highly active against some quinolone-resistant bacteria including quinolone-resistant MRSA. Preliminary studies indicated that oxoquinolizines possess distinct activity and toxicity profiles as compared with their parent quinolones. In order to develop a potent antibacterial agent with the desired spectrum of activity, good tolerability, and balanced pharmacokinetic profile, the authors synthesized and evaluated a series of oxoquinolizines with various substituents at the C-8 position I (NR1R2 = Q, Q1, Q2, etc.). Most compds. tested in this study demonstrated better activity against Gram-pos. bacteria than ciprofloxacin and exhibited good susceptibility against ciprofloxacin- and methicillin-resistant S. aureus. While maintaining potent in vitro activity, several compds. showed improved in vivo efficacy over ABT-719 as indicated by the mouse protection test. The current study revealed that the steric and electronic environment, conformation, and abs. stereochem. of the C-8 group are very important to the antibacterial profiles. Structural modifications of the C-8 group

provide a useful means to improve the antibacterial activities, physicochem. properties, and pharmacokinetic profiles. Manipulation of the C-8 group also allows us to generate analogs with the desired spectrum of activity, such as analogs that are selective against respiratory pathogens.

180975-96-6P 181141-54-8P 181141-55-9P 250274-71-6P 250274-72-7P 250274-75-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn., structure, bactericidal activity, and structure-activity relationship of oxoquinolizines)

RN 180975-96-6 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-, monohydrochloride, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 181141-54-8 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 181141-55-9 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 250274-71-6 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aR,6aS)-hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl]-9-methyl-4-oxo-, monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ H & & & \\ & & & \\ H & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\$$

RN 250274-72-7 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8[(4aR,7aR)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.

RN 250274-75-0 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8[(3aR,7aS)-octahydro-2H-pyrrolo[3,4-c]pyridin-2-yl]-4-oxo-,
monohydrochloride, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
ANSWER 10 OF 28 CAPLUS COPYRIGHT 2002 ACS
    1999:311055 CAPLUS
     130:338119
     Preparation of 7-substituted 3-hydroxyquinazoline-2,4-diones and related
     compounds as antibacterial agents.
IN
     Domagala, John Michael; Ellsworth, Edmund Lee; Huang, Liren; Renau, Thomas
     Eric; Singh, Rajeshwar; Stier, Michael Andrew
PA
     Warner Lambert Co., USA
     PCT Int. Appl., 137 pp.
SO
     CODEN: PIXXD2
DΤ
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                          APPLICATION NO. DATE
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                                          ______
                                                           -----
ΡI
     WO 9921840
                     A1
                           19990506
                                          WO 1998-US19877 19980923
         W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HR, HU, ID, IL,
             IS, JP, KP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL,
             RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG,
             KZ, MD, RU, TJ, TM
         RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES,
             FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI,
             CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
                      A1 19990517
A1 20000823
     AU 9895039
                                          AU 1998-95039
                                                            19980923
     EP 1028950
                                          EP 1998-948473
                                                           19980923
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO
     ZA 9809783
                            19990428
                                          ZA 1998-9783
                      Α
                                                            19981027
    US 6331538
                      В1
                            20011218
                                          US 2000-508796
                                                            20000315
    US 2002115674
                            20020822
                                          US 2001-971343
                      A1
                                                           20011004
PRAI US 1997-63556P
                      Ρ
                            19971028
    US 1998-98588P
                      Ρ
                            19980831
    WO 1998-US19877
                      W
                            19980923
    US 2000-508796
                      АЗ
                           20000315
OS
    MARPAT 130:338119
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AB Title compds. [I; R1 = H, (substituted) alkyl, cycloalkyl, heterocyclyl, Ph; R5, R6, R8 = H, F, Cl, Br, NO2, cyano, CF3, alkyl, cycloalkyl, amino, etc.; R7 = R5, (substituted) carbocyclyl, Ph, (fused) heterocyclyl, etc.; R1R8 = (substituted) 6-7 membered (heterocyclic) ring; X, Y = C, N], were prepd. Thus, 1-cyclopropyl-6-fluoro-3-hydroxy-7-(pyrrolidin-1-yl)-1H-quinazoline-2,4-dione (prepn. given) inhibited Staphylococcus aureus with min. inhibitory concn. = 1.0 .mu.g/mL.

IT 224189-79-1P

IT 224189-79-1P

RI: BAC (Biological activity or effector except

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

Relative stereochemistry.

CM 2

CRN 76-05-1

CMF C2 H F3 02

IT 224190-98-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of 7-substituted 3-hydroxyquinazoline-2,4-diones and related compds. as antibacterial agents)

RN 224190-98-1 CAPLUS

CN 2,4(1H,3H)-Quinazolinedione, 1-cyclopropyl-6-fluoro-7-[(4aR,7aR)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-3-(phenylmethoxy)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 11 OF 28 CAPLUS COPYRIGHT 2002 ACS AN 1998:665013 CAPLUS

DN 130:47161

TI In vivo efficacy of ABT-255 against drug-sensitive and -resistant Mycobacterium tuberculosis strains

AU Oleksijew, Andy; Meulbroek, Jon; Ewing, Patty; Jarvis, Ken; Mitten, Mike; Paige, Lenette; Tovcimak, Ann; Nukkula, Mike; Chu, Daniel; Alder, Jeffrey D.

CS Experimental Therapeutics and Pharmacology, Abbott Laboratories, Abbott Park, IL, 60064, USA

SO Antimicrobial Agents and Chemotherapy (1998), 42(10), 2674-2677 CODEN: AMACCQ; ISSN: 0066-4804

PB American Society for Microbiology

DT Journal

LA English

AΒ Current therapy for pulmonary tuberculosis involves 6 mo of treatment with isoniazid, pyrazinamide, rifampin, and ethambutol or streptomycin for reliable treatment efficacy. The long treatment period increases the probability of noncompliance, leading to the generation of multidrug-resistant isolates of Mycobacterium tuberculosis. A treatment option that significantly shortened the course of therapy, or a new class of antibacterial effective against drug-resistant M. tuberculosis would be of value. ABT-255 is a novel 2-pyridone antibacterial agent which demonstrates in vitro potency and in vivo efficacy against drug-susceptible and drug-resistant M. tuberculosis strains. By the Alamar blue redn. technique, the MIC of ABT-255 against susceptible strains of M. tuberculosis ranged from 0.016 to 0.031 .mu.g/mL. The MIC of ABT-255 against rifampin- or ethambutol-resistant M. tuberculosis isolates was 0.031 .mu.g/mL. In a murine model of pulmonary tuberculosis, 4 wk of oral ABT-255 therapy produced a 2- to 5-log10 redn. in viable drug-susceptible M. tuberculosis counts from lung tissue. Against drug-resistant strains of M. tuberculosis, ABT-255 produced a 2- to 3-log10 redn. in viable bacterial counts from lung tissue. ABT-255 is a promising new antibacterial agent with activity against M. tuberculosis.

IT 181141-52-6, ABT 255

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(in vivo efficacy of ABT-255 against drug-sensitive and -resistant Mycobacterium tuberculosis strains)

RN 181141-52-6 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-[(4as,7as)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RE.CNT 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 12 OF 28 CAPLUS COPYRIGHT 2002 ACS

AN 1998:565044 CAPLUS

DN 129:275852

TI Diastereoselective 1,3-dipolar cycloadditions with enantiopure azomethine ylides

AU Enders, Dieter; Meyer, Ilka; Runsink, Jan; Raabe, Gerhard

CS Inst. Organische Chem., Rheinisch-Westfalische Technische Hochschule, Aachen, D-52074, Germany

SO Tetrahedron (1998), 54(36), 10733-10752 CODEN: TETRAB; ISSN: 0040-4020

PB Elsevier Science Ltd.

DT Journal

LA English

OS CASREACT 129:275852

AB Secondary amine derivs. of (4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-amine, were heated with a variety of arom. aldehydes in chlorobenzene under reflux. The in situ generated 1,3-dipoles were trapped with fumaric acid ester, fumaric acid nitrile or N-phenylmaleimide, resp., that were present in excess in the reaction mixt. The cycloadducts were formed in 78-91% and 67-100% yield as mixt. of exo/endo-isomers (endo:exo = 30-65:70-35). These isomers were formed as diastereomerically pure compds. (de.gtoreq.96%).

IT 214079-35-3P 214079-36-4P

RN 214079-35-3 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, 2-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]octahydro-3-(4-methoxyphenyl)-4,6-dioxo-5-phenyl-, methyl ester, (1S,3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 214079-36-4 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, 2-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]octahydro-3-(4-methoxyphenyl)-4,6-dioxo-5-phenyl-, methyl ester, (1S,3S,3aS,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Absolute stereochemistry. Rotation (-).

RN 214079-30-8 CAPLUS
CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, 2-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]-3-(4-fluorophenyl)octahydro-4,6-dioxo-5-phenyl-, methyl ester, (1S,3S,3aS,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 214079-31-9 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, 2-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]octahydro-4,6-dioxo-3,5-diphenyl-, methyl ester, (1S,3S,3aR,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 214079-32-0 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, 2-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]octahydro-4,6-dioxo-3,5-diphenyl-, methyl ester, (1S,3S,3aS,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Page 98

RN 214079-33-1 CAPLUS

CN Pyrrolo[3,4-c].pyrrole-1-carboxylic acid, 3-(4-bromophenyl)-2-[(45,5s)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]octahydro-4,6-dioxo-5-phenyl-, methyl ester, (1s,3s,3aR,6as)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 214079-34-2 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1-carboxylic acid, 3-(4-bromophenyl)-2-[(45,5s)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]octahydro-4,6-dioxo-5-phenyl-, methyl ester, (1s,3s,3as,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 214079-37-5 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,3(2H,3aH)-dione, 5-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]tetrahydro-2,4,6-triphenyl-, (3aR,4S,6S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 214079-38-6 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,3(2H,3aH)-dione, 5-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]tetrahydro-2,4-diphenyl-, (3aR,4S,6aS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 214079-39-7 CAPLUS

CN Pyrrolo[3,4-c]pyrrole-1,3(2H,3aH)-dione, 5-[(4S,5S)-2,2-dimethyl-4-phenyl-1,3-dioxan-5-yl]tetrahydro-2,4-diphenyl-, (3aS,4S,6aR)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RE.CNT 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

ANSWER 13 OF 28 CAPLUS COPYRIGHT 2002 ACS 1998:15734 CAPLUS 128:102006 Process for preparation of chiral 3-aminopyrrolidine and analogous bicyclic compounds as intermediates for antibacterial agents ΙN Li, Qun; Wang, Wei-bo; Chu, Daniel T.; Hasvold, Lisa Anne PΑ Abbott Laboratories, USA SO U.S., 18 pp. CODEN: USXXAM DT Patent LΑ English FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. ____ ΡI US 5703244 Α 19971230 US 1996-754641 19961121 ZA 9709728 Α 19980522 ZA 1997-9728 19971029 TW 385230 В 20000321 TW 1997-86116224 19971030 WO 9822437 A1 19980528 WO 1997-US21081 19971118 W: AU, BG, BR, CA, CN, CZ, HU, IL, JP, KR, MX, NO, NZ, PL, RO, SI, SK, TR RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE AU 9873004 A1 19980610 AU 1998-73004 19971118 US 5837868 Α 19981117 US 1997-974206 19971119 PRAI US 1996-754641 Α 19961121 WO 1997-US21081 W 19971118 OS CASREACT 128:102006; MARPAT 128:102006 GΙ

CH₂Ar
$$H_2$$
N Me Me V

AB Claimed is a process for the prepn. of chiral 3-aminopyrrolidine (I; R = C1-6 alkyl, C2-6 alkenyl, C2-6 alkynyl, or C3-6 cycloalkyl; R1 = H, C1-6 alkyl or an amino-protecting group) and analogous bicyclic derivs. from dihydroxy olefins HOCH2CH:CHCH2OAr (Ar = aryl) by treatment with titanium isopropoxide, an optically active tartrate ester, and tert-Bu hydroperoxide, followed by subsequent alkylation of the intermediate (II;

Ar = aryl) with an alkyl or alkenyl magnesium halide to give HOCH2CHRCH(OH)CH2OCH2Ar (R = same as above), then formation of pyrrolidine ring (III; R, Ar = same as above) by condensation with an arylmethylamine, subsequent chiral replacement of a ring hydroxyl group with an amino group with further protection thereof, optional addnl. substitution closing of the second ring, and hydrogenolysis to remove a ring-nitrogen protecting The present invention describes an efficient process for the enantioselective prepn. of chiral 3-aminopyrrolidine, 2,7-diazabicyclo[3.3.0]octane, 2,8-diaza-bicyclo[4.3.0]nonane, and 2,9-diaza-bicyclo[5.3.0]decane derivs. which are useful as intermediates in the prepn. of certain pyrido[1,2-a]pyrimidine and quinolone antibacterial agents. Thus, (E)-4-benzyloxy-2-butene-1-ol was added dropwise to a stirred mixt. of di-Et L-(+)-tartrate and titanium isopropoxide in CH2Cl2 at -23.degree., followed by adding a soln. of tert-Bu hydroperoxide in decane at .apprx.-23.degree. to -30.degree. and the reaction mixt. was stored at -25.degree. overnight and stirred at .apprx.-23.degree. to -30.degree. for 7.5 h to give 83% (2S,3S)-3-(benzyloxymethyl)oxirane-2-methanol (IV). EtMgBr in THF was added to CuCN in Et20 at -50.degree. followed by adding a soln. of IV in Et20 at -50.degree. and the reaction mixt. was stirred at -50.degree. to -25.degree. for 4 h to give (2R,3R)-2-ethyl-4-benzyloxybutane-1,3-diol which was hydrogenolyzed over 10% Pd-C in EtOH at 4 atm H pressure at room temp. for $2\overline{4}$ h to give (2R,3R)-2-ethylpyrrolidine-1,3,4-triol. The latter compd. underwent Mitsunobu reaction with phthalimide, Ph3P, DEAD in THF followed by treatment with hydrazine, acylation with di-tert-Bu dicarbonate, and hydrogenolysis over Pd-C under H atm. to give (3S, 4R)-3-tert-butoxycarbonylamino-4-ethylpyrrolidine. Four quinolizine compds. were also prepd. and tested for antibacterial activity and for example, racemic V.HCl showed min. inhibitory concn. of 0.02 and 0.001 .mu.g/mL against Staphylococcus aureus ATCC 6538P and Escherichia coli Stainless Steel, resp.

TT 181141-52-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(process for prepn. of chiral aminopyrrolidine and analogous bicyclic compds. as intermediates for antibacterial agents)

RN 181141-52-6 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-[(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

HCl

IT 201228-12-8P 201228-20-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for prepn. of chiral aminopyrrolidine and analogous bicyclic compds. as intermediates for antibacterial agents)

RN 201228-12-8 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-8-[1-[(1,1-dimethylethoxy)carbonyl]octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-7-fluoro-9-methyl-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 201228-20-8 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-8-[1-[(1,1-dimethylethoxy)carbonyl]octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-7-fluoro-9-methyl-4-oxo-, ethyl ester, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

•

ANSWER 14 OF 28 CAPLUS COPYRIGHT 2002 ACS

AN 1997:594555 CAPLUS

DN 127:288165

TI Antitumor compounds

IN Tomita, Kyoji; Chiba, Katsumi; Kashimoto, Shigeki; Nakada, Katsuhisa; Shibamori, Koichiro; Chikugi, Yasutomo; Tajima, Masanori; Oue, Tomio

PA Dainippon Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 74 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

FAN.CNT 1

OS MARPAT 127:288165

GT

$$R^5$$
 R^4 R^3 R^4 R^3 R^4 R^3 R^4 R^4 R^3 R^4 R^4

AB The title compds. (I; X = N or C-Rx, with Rx =H, halogen; R1, R2 = H, halogen; R3 = H, carboxyl; R4 = oxo, OH; R5 = H, amino; R6 = substituted cyclic amino groups) and their physiol. acceptable salts are claimed as antitumor drugs. Thus, I were prepd., and their antitumor activities were tested in animal models.

IT 196821-69-9P 196821-73-5P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (antitumor compds.)

RN 196821-69-9 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-1-(2-thiazolyl)-, monohydrochloride, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 196821-73-5 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-1-(2-thiazolyl)-, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.

```
ANSWER 15 OF 28 CAPLUS COPYRIGHT 2002 ACS
     1997:116497 CAPLUS
     126:117990
     Preparation of quinolizinone- and pyridopyrimidinonecarboxylates as
     antibacterials
IN
     Chu, Daniel T.; Li, Qun; Cooper, Curt S.; Fung, Anthony K. L.; Lee, Cheuk
     M.; Plattner, Jacob J.; Ma, Zhenkun; Wang, Wei-Bo
PA
     Abbott Laboratories, USA
     PCT Int. Appl., 412 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 4
     PATENT NO.
                      KIND DATE
                                          APPLICATION NO.
                                                           DATE
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                                          -----
ΡI
     WO 9639407
                                          WO 1996-US8991
                      A1
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                            19961224
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                                                           19960605
     EP 871628
                      Α1
                           19981021
                                          EP 1996-919103
                                                           19960605
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, FI
     JP 11510478
                      T2
                            19990914
                                          JP 1996-501420
                                                           19960605
PRAI US 1995-469159
                      Α
                            19950606
    US 1996-638112
                      Α
                            19960529
    WO 1996-US8991
                      W
                            19960605
os
    MARPAT 126:117990
GΙ
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$$R^{3}$$
 R^{5}
 $CO_{2}R^{4}$
 R^{2}
 R^{1}
 R^{1}
 R^{2}
 R^{3}
 R^{5}
 R^{5}
 R^{6}
 R^{7}
 R^{7}

AB Title compds. [I; A = N or CR6; R1 = halo, (cyclo)alkyl, alkoxy, (un)substituted Ph, etc.; R2 = halo, (cyclo)alkyl, alkoxy, N-contg. heterocyclyl, etc.; R3 = H, halo, alkoxy; R4 = H, alkyl, cation, etc.; R5, R6 = H, halo, alkyl, alkoxy, etc.] were prepd. Thus, 4-FC6H4CH2C(:NH)NH2 was cyclocondensed with NaOCH:CFC02Et (prepn. given) and the chlorinated product aminated by 1-methylpiperazine to give 5-fluoro-2-(4-fluorobenzyl)-4-(4-methylpiperazino)pyrimidine which was condensed with EtOCH:C(C02Et)2 and the product cyclized to give, in 2 addnl. steps, title compd. II. Data for biol. activity of I were given. IT 169748-73-6P 181141-52-6P 181141-53-7P 181141-54-8P 181141-55-9P 185692-32-4P

● HCl

RN 181141-52-6 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-[(4as,7as)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

RN 181141-53-7 CAPLUS
CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride,
(4aR-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

HCl

RN 181141-54-8 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 181141-55-9 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 185692-32-4 CAPLUS
CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8(hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl)-9-methyl-, monohydrochloride
(9CI) (CA INDEX NAME)

Me N CO2H

● HCl

RN 185692-33-5 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

$$\stackrel{\text{He}}{\underset{\text{N}}{\bigvee}} \stackrel{\text{Me}}{\underset{\text{N}}{\bigvee}} co_2 H$$

● HCl

RN 185692-55-1 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-1-methyl-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 186196-97-4 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 186197-31-9 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl)-9-methyl-4-oxo- (9CI) (CA INDEX NAME)

RN 186197-32-0 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-

(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo- (9CI) (CA INDEX NAME)

RN 186197-48-8 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-9-methyl-4-oxo- (9CI) (CA INDEX NAME)

RN 186197-76-2 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-1-methyl-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo- (9CI) (CA INDEX NAME)

RN 186198-52-7 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-2H-pyrrolo[3,4-c]pyridin-2-yl)-4-oxo- (9CI) (CA INDEX NAME)

RN 186198-55-0 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl)-9-methyl-4-oxo-, (3aR-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 186198-56-1 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl)-9-methyl-4-oxo-, (3aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 186293-38-9 CAPLUS

CN* 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 186293-50-5 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aR-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

ANSWER 16 OF 28 CAPLUS COPYRIGHT 2002 ACS

1996:754424 CAPLUS 126:101707

ΤI Synthesis of quinolizinone-type antibacterial compounds

Chu, Daniel T.; Li, Qun; Cooper, Curt S.; Fung, Anthony K. L.; Lee, Cheuk M.; Plattner, Jacob J.

PA Abbott Laboratories, USA

SO U.S., 115 pp., Cont.-in-part of U.S. Ser. No. 137,236, abandoned. CODEN: USXXAM

DΤ Patent

LΑ English

FAN. CNT 4

T. TATA	CNI 4						
	PATENT NO.		DATE	APPLICATION NO.	DATE		
PΙ	US 5580872	Α	19961203	US 1994-316319	19940930		
	US 5599816	Α	19970204	US 1995-482249	19950607		
	US 5726182	Α	19980310	US 1995-484632	19950607		
PRAI	US 1990-517780	B2	19900502				
	US 1992-940870	B2	19921027				
	US 1993-137236	B2	19931014				
	US 1994-316319	A2	19940930				
	US 1995-469159	A 3	19950606				
OS	MARPAT 126:101707	7					
GT							

$$R^3$$
 R^5
 CO_2R^4
 R^2

Antibacterial quinolizinones and related compds. [I; R1 = (halo)alkyl, alkenyl, alkynyl, alkoxy, C3-8 cycloalkyl, (substituted) Ph, halo, CN, NO2, bicycloalkyl, N-contg. arom. heterocyclyl, etc.; R2 = alkyl, alkenyl, C3-8 cycloalkyl, C4-8 cycloalkenyl, NH2, :NH, alkylamino, (substituted) Ph, N-contg. bicyclic or arom. heterocyclyl, etc.; R3 = H, halo, alkoxy; R4 = H, alkyl, cation, prodrug ester group; R5 = H, halo, OH, alkyl, haloalkyl, alkoxy, (substituted) amino; A = N, CR6; R6 = halo, (substituted) alkyl, alkoxy] are prepd. for use in pharmaceutical compns. for treatment of bacterial infections. Thus, 3-fluoro-9-(4-fluorophenyl)-2-(4-methylpiperazin-1-yl)-6H-6-oxopyrido[1,2-a]pyrimidine-7-carboxylic acid (II) showed a MIC of 0.39 and 0.1 .mu.g/mL in vitro against Staphylococcus aureus A5177 and Pseudomonas aeruginosa BMH10, resp. II was prepd. in 6 steps from 5-fluoro-2-(4-fluorobenzyl)-4-hydroxypyrimidine (prepn. given).

ΙT 185692-32-4P 185692-33-5P 185692-55-1P

Ι

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(synthesis of quinolizinone-type antibacterial compds.)

RN 185692-32-4 CAPLUS

4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-

09/833,914

(hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl)-9-methyl-, monohydrochloride
(9CI) (CA INDEX NAME)

● HCl

RN 185692-33-5 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 185692-55-1 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-1-methyl-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

09/833,914 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2002 ACS 1996:596103 CAPLUS 125:247794 Preparation of novel pyridonecarboxylic acid derivatives or their salts as antibacterial agents IN Yazaki, Akira; Yoshida, Jiro; Niino, Yoshiko; Ohshita, Yoshihiro; Hayashi, Norihiro; Amano, Hirotaka; Hirao, Yuzo; Kuramoto, Yasuhiro PΑ Wakunaga Seiyaku Kabushiki Kaisha, Japan PCT Int. Appl., 222 pp. CODEN: PIXXD2 DTPatent LΑ Japanese FAN.CNT 2 PATENT NO. KIND DATE APPLICATION NO. DATE ----------A1 19960808 WO 1996-JP152 19960126 W: AU, BR, CA, CN, HU, JP, KR, MX, RU, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE CA 2211681 AA 19950130 CA 1996-2211681 19960126 AU 9652600 A1 19960821 AU 1996-52600 19960126 PRAI JP 1995-12673 19950130

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

19960126

- AB Pyridonecarboxylic acid derivs. [I; R1 = H, protecting group; R2 = NO2, (un)substituted NH2; R3 = halo; R4, R5 = H, halo, alkyl, alkoxy; R6 = H, halo, OH, alkyl, amino; R7 = H, halo; A = N, CX (wherein X = H, halo, alkyl, alkoxy); Z = halo, (un)substituted satd. cyclic amino], broad-spectrum bactericides with extremely low toxicity, are prepd. A mixt. of chloro compd. II, (3S)-3-aminopyrrolidine, and Et3N in DMF was heated with stirring at 90.degree., the mixt. was cooled, dissolved in EtOH and refluxed to give (S)-pyrrolidinyl compd. III, which showed MIC of 0.025 .mu.g/mL against S. aureus 209P, vs. 0.05 with tosufloxacin.
- IT 179741-45-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of novel pyridonecarboxylic acid derivs. or their salts as antibacterial agents)

RN 179741-45-8 CAPLUS

WO 1996-JP152

GΙ

MARPAT 125:247794

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(5-amino-2,4-difluorophenyl)-6-fluoro-7-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-1,4-dihydro-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

```
ANSWER 18 OF 28 CAPLUS COPYRIGHT 2002 ACS
   1996:574482 CAPLUS
    125:221832
DN
     Preparation of derivatives of 1,6-naphthyridinecarboxylic acids as
TI
     antibacterials.
    Bartel, Stephan; Grohe, Klaus; Hagemann, Hermann; Bremm, Klaus-Dieterr;
    Endermann, Rainer
PΑ
    Bayer A.-G., Germany
    Eur. Pat. Appl., 54 pp.
SO
    CODEN: EPXXDW
DΤ
    Patent
LA
    German
FAN.CNT 1
                                       APPLICATION NO. DATE
    PATENT NO.
                   KIND DATE
                          -----
     -----
                                         -----
    EP 726270 A1 19960814
EP 726270 B1 20010523
                                       EP 1996-101170 19960129
PΙ
       R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
    DE 19506535 Al 19960814 DE 1995-19506535 19950224
    ES 2158963
                    T3 20010916
                                        ES 1996-101170 19960129
    JP 08253480 A2 19961001
CA 2168921 AA 19960810
US 5811433 A 19980922
                                        JP 1996-40599
                                                         19960202
                                        CA 1996-2168921 19960206
                                        US 1997-878683 19970619
PRAI DE 1995-19504280 A 19950209
    DE 1995-19506535 A
                         19950224
    US 1996-595603 B1 19960202
    MARPAT 125:221832
GΙ
```

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB Title compds. [I; R1 = (substituted) alkyl, cycloalkyl, alkenyl, alkoxy, amino, Ph; R2 = H, (substituted) alkyl, (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl; X1 = H, halo, Me, CF3; Z = Q1-Q3; R3 = H, OH, amino, CH2OH, aminomethyl; R4 = H, alkyl, cyclopropyl; R41 = H, Me], were prepd. Thus, 7,8-dichloro-1-cyclopropyl-1,4-dihydro-4-oxo-1,6-naphthyridin-3-carboxylic acid (prepn. given) and (3a.alpha.,4.beta.,7.beta.,7a.alpha.)-4-amino-7-methyl-1,3,3a,4,7,7a-hexahydroisoindole were refluxed 6 h in MeCN/DMF to give 82% title compd. (II). II showed a min. inhibitory concn. of 0.25.mu.g/mL.
- IT 181261-32-5P 181261-65-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of derivs. of 1,6-naphthyridinecarboxylic acids as antibacterials)

RN 181261-32-5 CAPLUS

CN 1,6-Naphthyridine-3-carboxylic acid, 8-chloro-1-cyclopropyl-7-(1,4,4a,5,7,7a-hexahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-1,4-dihydro-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 181261-65-4 CAPLUS

CN 1,6-Naphthyridine-3-carboxylic acid, 8-chloro-1-(2-fluorocyclopropyl)-7-(1,4,4a,5,7,7a-hexahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-1,4-dihydro-5-methyl-4-oxo-, [4aS-[4a.alpha.,6(1S*,2R*),7a.alpha.]]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

ANSWER 19 OF 28 CAPLUS COPYRIGHT 2002 ACS

M. 1996:485623 CAPLUS

125:142699

TI Preparation of novel quinoline- and naphthyridinecarboxylate derivatives as antibacterial agents

IN Yazaki, Akira; Yoshida, Jiro; Niino, Yoshiko; Ohshita, Yoshihiro; Hayashi, Norihiro; Amano, Hirotaka; Hirao, Yuzo; Kuramoto, Yasuhiro

PA Wakunaga Seiyaku Kabushiki Kaisha, Japan

SO PCT Int. Appl., 221 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

FAN. CNT 2

CNT	2															
PA'	rent :	NO.		KIND	DATE			AP	PLIC	ATIC	ои ис).	DATE			
												-				
WO	9612	704		A1	19960	502		WO	199	5-JI	P2156	5	1995	1020		
	W:	JP,	US													
	RW:	ΑT,	BE,	CH, DE	, DK,	ES,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE
EP	7877	20		A1	19970	806		EP	199	5-93	34853	}	1995	1020		
	R:	DE,	FR,	GB												
US	5910	498		Α	19990	608		US	199	7-81	17603	}	1997	0708		
JΡ	1994	-2550	046		19941	.020										
JΡ	1995	-126	73		19950	130										
WO	1995	-JP2	156		19951	020										
MAI	RPAT	125:	14269	99												
	PA'	WO 9612 W: RW: EP 7877 R: US 5910 JP 1994 JP 1995 WO 1995	PATENT NO	PATENT NO	PATENT NO. KIND	PATENT NO. KIND DATE AP	PATENT NO. KIND DATE APPLICATION OF THE PATENT NO. CONTROL OF THE PATENT NO. CON	PATENT NO. KIND DATE APPLICATION WO 9612704 A1 19960502 WO 1995-JM W: JP, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, EP 787720 A1 19970806 EP 1995-93 R: DE, FR, GB US 5910498 A 19990608 US 1997-83 JP 1994-255046 19941020 JP 1995-12673 19950130 WO 1995-JP2156 19951020	PATENT NO. KIND DATE APPLICATION NO. WO 9612704 Al 19960502 WO 1995-JP2156 W: JP, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, EP 787720 Al 19970806 EP 1995-934853 R: DE, FR, GB US 5910498 A 19990608 US 1997-817603 JP 1994-255046 19941020 JP 1995-12673 19950130 WO 1995-JP2156 19951020	PATENT NO. KIND DATE APPLICATION NO. WO 9612704 A1 19960502 WO 1995-JP2156 W: JP, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, EP 787720 A1 19970806 EP 1995-934853 R: DE, FR, GB US 5910498 A 19990608 US 1997-817603 JP 1994-255046 19941020 JP 1995-12673 19950130 WO 1995-JP2156 19951020	PATENT NO. KIND DATE APPLICATION NO. DATE WO 9612704 A1 19960502 WO 1995-JP2156 1995 W: JP, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, EP 787720 A1 19970806 EP 1995-934853 1995 R: DE, FR, GB US 5910498 A 19990608 US 1997-817603 19970 JP 1994-255046 19941020 JP 1995-J2673 19950130 WO 1995-JP2156 19951020	PATENT NO. KIND DATE APPLICATION NO. DATE WO 9612704 Al 19960502 WO 1995-JP2156 19951020 W: JP, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, EP 787720 Al 19970806 EP 1995-934853 19951020 R: DE, FR, GB US 5910498 A 19990608 US 1997-817603 19970708 JP 1994-255046 19941020 JP 1995-J2673 19950130 WO 1995-JP2156 19951020	PATENT NO. KIND DATE APPLICATION NO. DATE WO 9612704 Al 19960502 WO 1995-JP2156 19951020 W: JP, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, EP 787720 Al 19970806 EP 1995-934853 19951020 R: DE, FR, GB US 5910498 A 19990608 US 1997-817603 19970708 JP 1994-255046 19941020 JP 1995-J2673 19950130 WO 1995-JP2156 19951020			

AB The title compds. [I; R1 = H, protecting group; R2 = NO2, (substituted) amino; R3 = halo; R4, R5 = H, halo, alkyl, alkoxy; A = N, CX (wherein X = H, halo, alkyl, alkoxy); Z = halo, (substituted) satd. cyclic amino group], effective broad-spectrum antibacterial agents, are prepd. Nitration of 2.00 g difluorophenyl compd. II (R2 = H) with KNO3/H2SO4 at room temp. gave 2.08 g nitro compd. II (R2 = NO2). Some I showed MIC as low as <0.013 .mu.g/mL against S. aureus, vs. 0.05 .mu.g/mL with tosufloxacin.

IT 179741-45-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of novel quinoline- and naphthyridinecarboxylate derivs. as

antibacterial agents) 179741-45-8 CAPLUS

RN

1,8-Naphthyridine-3-carboxylic acid, 1-(5-amino-2,4-difluorophenyl)-6-fluoro-7-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-1,4-dihydro-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME) CN

HCl

8 AN

ANSWER 20 OF 28 CAPLUS COPYRIGHT 2002 ACS

1996:422678 CAPLUS

N 125:221511

TI Synthesis and Structure-Activity Relationships of 2-Pyridones: A Novel Series of Potent DNA Gyrase Inhibitors as Antibacterial Agents

AU Li, Qun; Chu, Daniel T. W.; Claiborne, Akiyo; Cooper, Curt S.; Lee, Cheuk M.; Raye, Kathleen; Berst, Kristine B.; Donner, Pamela; Wang, Weibo; et al.

CS Abbott Laboratories, Abbott Park, IL, 60064-3500, USA

SO Journal of Medicinal Chemistry (1996), 39(16), 3070-3088

CODEN: JMCMAR; ISSN: 0022-2623

PB American Chemical Society

DT Journal

LA English

GΙ

$$H_2N$$
. Me CO_2H

AB Two novel series of 2-pyridones, e.g. I (R = 2, 4-F2C6H3), II, were synthesized by transposition of the nitrogen of 4-quinolones to the bridgehead position. This subtle interchange of the nitrogen atom with a carbon atom yielded two novel heterocyclic nuclei, pyrido[1,2-a]pyrimidine and quinolizine, which had not previously been evaluated as antibacterial agents and were found to be potent inhibitors of DNA gyrase. Quinolizines with a Me group at the 9-position such as II (ABT-719) demonstrate exceptional broad spectrum antibacterial activity. Most notably, they are active against resistant bacteria such as methicillin-resistant Staphylococcus aureus, vancomycin-resistant strains of enterococci, and ciprofloxacin-resistant organisms. In addn., 2-pyridones also possess favorable physiochem. and pharmacokinetic properties. These 2-pyridones were synthesized from the com. available starting materials by 10-17linear transformations. The structure of an adduct yielded by this sequence, ABT-719, was detd. by X-ray crystallog. anal.

IT 180975-95-5P 180975-96-6P 181141-52-6P 181141-53-7P 181141-54-8P 181141-55-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(prepn. and bactericidal activity of 2-pyridones)

RN 180975-95-5 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, dihydrochloride, cis-(9CI) (CA INDEX NAME)

Relative stereochemistry.

●2 HCl

RN 180975-96-6 CAPLUS
CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-, monohydrochloride, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 181141-52-6 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8- [(4aS,7aS)-octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

● HCl

RN 181141-53-7 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-9-methyl-8-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride, (4aR-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

● HCl

RN 181141-54-8 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aS,6aS)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 181141-55-9 CAPLUS

CN 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-[(3aR,6aR)-hexahydropyrrolo[3,4-b]pyrrol-5(1H)-yl]-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

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ANSWER 21 OF 28 CAPLUS COPYRIGHT 2002 ACS
    1995:892832 CAPLUS
DN
     123:313930
     Preparation of quinolizinonecarboxylates and analogs as antibacterials
     Chu, Daniel T.; Li, Qun; Cooper, Curt S.; Fung, Anthony K. L.; Lee, Cheuk
     M.; Plattner, Jacob J.
     Abbott Laboratories, USA
PΑ
     PCT Int. Appl., 255 pp.
SO
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 4
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                             DATE
                      ____
                                           ---------
PΙ
     WO 9510519
                            19950420
                       Α1
                                           WO 1994-US11166 19940930
         W: AU, BR, CA, CN, JP, KR
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
    AU 9479258
                                           AU 1994-79258
                                                             19940930
                       A1
                            19950504
    AU 689809
                       B2
                            19980409
     EP 723545
                       A1
                            19960731
                                           EP 1994-929998
                                                             19940930
    EP 723545
                       В1
                            20020508
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
    CN 1137273
                            19961204
                                           CN 1994-194479
                       Α
                                                             19940930
     CN 1053188
                       В
                            20000607
     JP 09503783
                       T2
                            19970415
                                           JP 1994-511876
                                                             19940930
    BR 9407806
                       Α
                            19970819
                                           BR 1994-7806
                                                             19940930
    AT 217309
                       Ε
                            20020515
                                           AT 1994-929998
                                                             19940930
PRAI US 1993-137236
                       Α
                            19931014
    WO 1994-US11166
                       W
                            19940930
OS
    MARPAT 123:313930
GΙ
```

AB Title compds. [I; R1 = halo, (cyclo) alkyl, Ph, heterocyclyl, etc.; R2 = halo, (cyclo)alk(en)yl, Ph, heterocyclyl, etc.; R3 = H, halo, alkoxy; R4 = H, alkyl, cation, ester residue; R5 = H, halo, OH, alkyl, etc.; R6 = alkyl] were prepd. Thus, 3-chlorotetrafluoropyridine was converted in a multistep synthesis to 2-(4-chloro-5-fluoro-3-methyl-2-pyridyl)cyclopropaneacetaldehyde which was condensed with CH2(CO2Et)2 and the product cyclized to give, after amination, title compd. (R)-II.HCl [R = (S)-CH(NH2)Et] which had MIC of 0.05 and 12.5.mu.g/mL against Staphylococcus aureus 1775 and Candida albicans CCH 442, resp.

Page 128

RN

CN

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of quinolizinonecarboxylates and analogs as antibacterials) 169748-73-6 CAPLUS 4H-Quinolizine-3-carboxylic acid, 1-cyclopropyl-7-fluoro-8-(hexahydropyrrolo[3,4-c]pyrrol-2(1H)-yl)-9-methyl-4-oxo-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

ANSWER 22 OF 28 CAPLUS COPYRIGHT 2002 ACS

AN 1995:408383 CAPLUS

122:290876

TI Preparation of penemylmethyl and cephalosporinylmethyl 7-(diazabicyclonono)quinolonecarboxylates as bactericides

IN Petersen, Uwe; Schroeck, Wilfried; Haebich, Dieter; Krebs, Andreas; Schenke, Thomas; Phillipps, Thomas; Grohe, Klaus; Endermann, Rainer; Bremm, Klaus Dieter; Metzger, Karl Georg

PA Bayer A.-G., Germany

χ2

0

SO Ger. Offen., 46 pp.

CODEN: GWXXBX

DT Patent

LA German

FAN.CNT 1

GI

FAN.CNT I								
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
PI	DE 4234330	A1	19940414	DE 1992-4234330	19921012			
	EP 592868	A1	19940420	EP 1993-115705	19930929			
	R: AT, BE,	CH, DE	, DK, ES, FR,	GB, GR, IE, IT, LI	, LU, MC, NL, PT, SE			
	CA 2108060	AA	19940413		19931008			
	JP 06228154	A2	19940816	JP 1993-277331	19931012			
PRAI	DE 1992-4234330		19921012					
os	MARPAT 122:29087	6						

AB Title compds. [I; A = N, CR3; B = O or S; L = (carba)penemylmethyl group Q1, cephalosporinylmethyl group Q2; R = diazabicyclonono group Q; R1 = (cyclo)alkyl, alkenyl, (fluoro)phenyl, OMe, NH2, etc.; R2 = H, Me, Et, alkoxycarbonyl, etc.; R3 = H, halo, Me, alkenyl, alkynyl, OH, OMe; R1R3 = Z1CH2CHMe, OCH2NR4; R4 = H, Me, CHO; R5 = H, CH2Ph, alkyl, etc.; R6 = H, OMe; R7 = H, acyl, alkoxycarbonyl, etc.; X1 = halo; X2 = H, halo, Me, (di)(alkyl)amino, OH, alkoxy, etc.; Y = CH2, CHMe, S; Z = CH2 or O; Z1 = O, S, CH2] were prepd. as bactericides (no data). Thus, Cs 1-cyclopropyl-7-[(1S,6S)-2-tert-butoxycarbonyl-2,8-diazabicyclo[4.3.0]non-8-yl]-6,8-difluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylate was condensed with benzhydryl (6R,7R)-7-phenylacetylamino-3-chloromethyl-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-ene-2-carboxylate to give, after deprotection, (6R,7R)-2-carboxy-8-oxo-7-phenylacetylamino-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-ylmethyl 1-cyclopropyl-7-[(1S,6S)-2,8-diazabicyclo[4.3.0]non-8-yl]-6,8-difluoro-1,4-dihydro-4-oxo-3-quinolinecarboxylate.

09/833,914

IT 151095-98-6P 151096-11-6P 161594-38-3P 161594-46-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. of penemylmethyl and cephalosporinylmethyl 7-(diazabicyclonono)quinolonecarboxylates as bactericides)

RN 151095-98-6 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 151096-11-6 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, ethyl ester, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 161594-38-3 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, hydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

●x HCl

RN 161594-46-3 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, hydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

●x HCl

LIR ANSWER 23 OF 28 CAPLUS COPYRIGHT 2002 ACS AN 1994:630582 CAPLUS

DN 121:230582

TI Quinolonecarboxylic acid .beta.-lactam antibiotics

IN Petersen, Uwe; Schroeck, Wilfried; Haebich, Dieter; Krebs, Andreas; Schenke, Thomas; Philipps, Thomas; Grohe, Klaus; Endermann, Rainer; Bremm, Klaus Dieter; Metzger, Karl Georg

PA Bayer A.-G., Germany

SO Eur. Pat. Appl., 82 pp.

CODEN: EPXXDW

DT Patent

LA German

FAN. CNT 1

GΙ

FAN.CNT 1								
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE			
ΡI	EP 591808	A1	19940413	EP 1993-115565	19930927			
	R: AT, BE, C	CH, DE	, DK, ES, H	FR, GB, GR, IE, IT, LI,	LU, MC, NL, PT, SE			
	DE 4234078	A1	19940414	DE 1992-4234078	19921009			
	NO 9303393	Α	19940411	NO 1993-3393	19930923			
	AU 9348644	A1	19940421	AU 1993-48644	19930927			
	AU 666772	B2	19960222					
	US 5480879	Α	19960102	US 1993-13Ì253	19931001			
	CA 2107812	AA	19940410	CA 1993-2107812	19931006			
	FI 9304411	Α	19940410	FI 1993-4411	19931007			
	ZA 9307474	Α	19940426	ZA 1993-7474	19931008			
	HU 66376	A2	19941128	HU 1993-2843	19931008			
	JP 08020587	A2	19960123	JP 1993-277526	19931008			
	CN 1090285	Α	19940803	CN 1993-118514	19931009			
PRAI	DE 1992-4234078		19921009					
os	MARPAT 121:230582	2						

$$X^{2}$$
 $CO_{2}R^{2}$
 $CO_{2}R^{2}$

AB The title compd. [I; A = N, (un)substituted CH; R1 = C1-4 alkyl, C2-4 alkenyl, C3-6 cycloalkyl, dicyclo[1.1.1]pent-1-yl, etc.; R2 = H, (un)substituted C1-5 alkyl, or (5-methyl-2-oxo-1,3-dioxol-4-yl)methyl; X1 = halogen; X2 = H, amino, alkylamino, dialkylamino, etc.; Z = 26-lactam

II

Ι

residue-contg. (un)substituted substituent], useful as antibiotics for the treatment of bacterial infections, are prepd. Thus, .beta.-lactam II was prepd. and demonstrated min. inhibitory concn. against Staphylococcus aureus (ICB 25701) of 0.25 .mu.g/mL.

IT 151095-98-6P 151096-11-6P 151096-12-7P 158182-91-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(prepn. and reaction of, in prepn. of antibiotics)

RN 151095-98-6 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 151096-11-6 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, ethyl ester, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 151096-12-7 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

RN 158182-91-3 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

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ANSWER 24 OF 28 CAPLUS COPYRIGHT 2002 ACS
    1994:605332 CAPLUS
     121:205332
TΙ
     Preparation of quinoline-derivative antibiotics
     Kim, Wan Joo; Park, Tae Ho; Kim, Bong Jin; Kim, Moon Hwan; Pearson, Neil
     Korea Research Institute of Chemical Technology, S. Korea; SmithKline
     Beecham PLC
     PCT Int. Appl., 47 pp.
     CODEN: PIXXD2
DT
     Patent
LΑ
     English
FAN.CNT 1
     PATENT NO.
                      KIND DATE
                                           APPLICATION NO.
                                                            DATE
                      ----
     WO 9415938
                           19940721
                      A1
                                           WO 1994-KR5
                                                            19940118
        W: AU, CA, CN, JP, NZ, US
         RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
     AU 9458665
                       A1
                            19940815
                                           AU -1994-58665
                                                            19940118
     EP 690862
                                           EP 1994-904771
                       Α1
                            19960110
                                                            19940118
     EP 690862
                      В1
                            20020710
        R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
     JP 08505385
                       T2
                            19960611
                                           JP 1994-515886
                                                            19940118
     AT 220401
                       E
                            20020715
                                           AT 1994-904771
                                                            19940118
     US 5770597
                       Α
                            19980623
                                           US 1995-492086
                                                            19951011
PRAI KR 1993-543
                       Α
                            19930118
    WO 1994-KR5
                       W
                            19940118
OS
    MARPAT 121:205332
GΙ
```

AB The title compds. [I; A = N, (Y)C:; Y = H, halogen, alkyl, alkoxy, etc.; R1 = (un)substituted C1-3 alkyl or cycloalkyl; R2 = H, lower alkyl; X1 = H, NH2, alkyl, halogen; X2 = H. halogen; Y1, Y2 = H, lower alkyl], useful as broad-spectrum antibiotics, are prepd. Thus, 1-cyclopropyl-6-fluoro-7-[(trans-piperidinopyrrolidine)-8-yl]-8-chloro-1,4-dihydroquinoline-4-oxo-3-carboxylic acid was prepd. and demonstrated MIC against Streptococcus pyogenes (308A) of 0.391 .mu.g/mL, vs. 3.125 .mu.g/mL for ciprofloxacin.

IT 157992-59-1 157992-62-6 158060-79-8

Ι

IT 157992-59-1 157992-62-6 158060-79-8 158060-80-1

RL: RCT (Reactant); RACT (Reactant or reagent)
 (antibiotic)

RN 157992-59-1 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-2-methyl-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo- (9CI) (CA INDEX NAME)

$$HO_2C$$
 HO_2C
 F

RN 157992-62-6 CAPLUS

CN 1,8-Naphthyridin-4(1H)-one, 1-(2,4-difluorophenyl)-6-fluoro-3-(nitroacetyl)-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-, monohydrochloride, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

RN 158060-79-8 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 158060-80-1 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

ANSWER 25 OF 28 CAPLUS COPYRIGHT 2002 ACS ► 1994:164147 CAPLUS 120:164147 TI Preparation of novel quinolone derivative or salt thereof and antibacterial agent containing the same Kuramoto, Yasuhiro; Noda, Shuichiro; Maruyama, Shinobu; Hatono, Shunso; IN Mochizuki, Haruyo; Yazaki, Akira PΑ Wakunaga Seiyaku K. K., Japan; Fujisawa Pharmaceutical Co., Ltd. PCT Int. Appl., 161 pp. CODEN: PIXXD2 DTPatent LΑ Japanese FAN.CNT 1 PATENT NO. KIND DATE APPLICATION NO. DATE ----WO 9313091 A1 19930708 WO 1992-JP1712 19921225 W: CA, JP, KR, US RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE EP 596126 A1 19940511 EP 1993-900445 19921225 R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE US 5412098 19950502 US 1993-104137 19930819 A PRAI JP 1991-346577 19911227 WO 1992-JP1712 19921225 OS MARPAT 120:164147 GΙ

Ι

AΒ Heterocyclylquinolone derivs. [I; R1 = H, CO2H-protecting group; R2 = H, halo, lower alkyl; X = H, halo; Y = halo, (un) substituted cyclic amino or cycloalkenyl, R3(CH2)mA; R3 = H, (un)substituted NH2; A = O, S; m = 0-3; Z = N, CR4; R4 = H, halo; W = (un)substituted 5-membered heterocyclyl having 3.gtoreq. hetero atoms including at least 2 N atoms], having potent antibacterial activity with low toxicity and high oral absorbability through oral administration and useful as human and animal drugs, medicines for fish, agrochems., and food preservatives, are prepd. Thus, 7-chloro-6-fluoro-1-(1,2,5-thiadiazol-3-yl)-1,4-dihydro-4-oxo-1,8naphthyridine-3-carboxylic acid 1.5, 3-(S)-aminopyrrolidine 0.46, and Et3N 1.06 g were stirred at 80.degree. in MeCN for 1 h to give, after workup and crystn. from EtOH, 1.5 g 7-[3-(S)-aminopyrrolidin-1-yl]-6-fluoro-1-(1,2,5-thiadiazol-3-yl)-1,4-dihydro-4-oxo-1,8-naphthyridine-3-carboxylic acid (II). II showed min. inhibitory concn. of <0.013, 0.2, and 0.1 .mu.g/mL against Escherichia coli NIH JC-2, Staphylococcus aureus 209P, and Pseudomonas aeruginosa, resp. A total of 229 I were prepd. 152513-85-4P 152613-25-7P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of, as antibacterial agent) RN 152513-85-4 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-1-(1,2,5-thiadiazol-3-yl)-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 152613-25-7 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 6-fluoro-1,4-dihydro-4-oxo-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-1-(1,2,5-thiadiazol-3-yl)-, monohydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

● HCl

```
ANSWER 26 OF 28 CAPLUS COPYRIGHT 2002 ACS
        ■ 1994:8616 CAPLUS
        Preparation of (diazabicyclononyl) quinolones and related compounds as
           antibacterials
IN
          Petersen, Uwe; Krebs, Andreas; Schenke, Thomas; Philipps, Thomas; Grohe,
           Klaus; Bremm, Klaus dieter; Endermann, Rainer; Metzger, Karl Georg;
          Haller, Ingo
          Bayer A.-G., Germany
PΑ
          Eur. Pat. Appl., 68 pp.
           CODEN: EPXXDW
DT
          Patent
LΑ
          German
FAN.CNT 1
          PATENT NO.
                                          KIND DATE
                                                                                      APPLICATION NO. DATE
       EP 550903 A1 19930714 EP 1992-122058 19921228
PΙ
               R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE
        DE 4200414 A1 19930715 DE 1992-4200414 19920110
DE 4208789 A1 19930923 DE 1992-4208789 19920319
DE 4208792 A1 19930923 DE 1992-4208792 19920319
NO 9204978 A 19930712 NO 1992-4978 19921222
CZ 289076 B6 20011017 CZ 1992-3966 19921229
A2 19931019 JP 1993-15917 19930105
AU 9331054 A1 19930715 AU 1993-31054 19930106
AU 669502 B2 19960613
CA 2086914 AA 19930711 CA 1993-2086914 19930107
IL 104331 A1 19970110 IL 1993-104331 19930107
IL 040351 A1 19970110 JI 1993-125 19930108
HU 64065 A2 19931129 HU 1993-34 19930108
HU 219488 B 20010428
PL 174853 B1 19980930 PL 1993-297338 19930108
PL 175558 B1 19980930 PL 1993-297338 19930108
PL 175558 B1 19990129 PL 1993-320107 19930108
CN 1074218 A 19930714 CN 1993-100215 19930109
CN 1043142 B 19990428
RU 2105770 C1 19980227 RU 1993-4405 19930110
FI 9701012 A 19970311 FI 1997-1012 19970311
CN 1192440 A 19980909 CN 1997-108773 19970201
CN 1061351 B 20010131
CN 1212256 A 19990331 CN 1998-109504 19980529
CN 1075499 B 20011128
FI 9900207 A 19990203 FI 1999-207 19990203
FI 2002000059 A 20020111 FI 2002-59 20020111
DE 1992-4208789 1 19920100
          DE 4200414 A1 19930715 DE 1992-4200414 19920110 DE 4208789 A1 19930923 DE 1992-4208789 19920319
PRAI DE 1992-4200414 A 19920110
          DE 1992-4208789 A 19920319
          DE 1992-4208792 A 19920319
          FI 1993-49 A 19930107
IL 1993-90940 A3 19930107
OS
         MARPAT 120:8616
GΙ
```

F CO₂H

$$R^{3}N$$
 $R^{4}N$
 $R^{4}N$
 $R^{4}N$
 $R^{3}N$
 $R^{4}N$
 R^{4

AB Title compds. [I; A = CH, CF, CCl, COMe, CMe, N; X1 = H, halo, NH2, Me; R1
= alkyl, FCH2CH2, cyclopropyl, (halo)phenyl; AR1 = COCH2CHMe; R2 = H,
 (substituted) alkyl, 5-methyl-2-oxo-1,3-dioxol-4-ylmethyl; B = Q1-Q3,
 etc.; Y = O, CH2; R3 = oxoalkyl, CH2COPh, R5O2CCH:CCO2R5, CH2CH2CO2R5,
 CH:CHCO2R5, CH2CH2CN; R4 = H, alkyl, 5-methyl-2-oxo-1,3-dioxol-4-ylmethyl,
 oxoalkyl, CH2COPh, CH2CH2CO2R5, R5O2CCH:CCO2R5, CH:CHCO2R5, CH2CH2CN; R5 =
 H, alkyl], were prepd. Thus, 1-cyclopropyl-6,7,8-trifluoro-1,4-dihydro-4 oxo-3-quindolinecarboxylic acid, 1,4-diazabicyclo[2.2.2]octane, and
 (+)-[S,S]-2,8-diazabicyclo[4.3.0]nonane (prepn. given) were refluxed in
 DMF to give 84% title compd. II. I were effective against Staph. aureus
 in mice at 2.5-10 mg/kg orally, vs. 80 mg/kg orally for ciprofloxacin.

IT 151095-98-6P 151096-11-6P 151096-12-7P 151096-27-4P 151213-20-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses) (prepn. of, as antibacterial)

RN 151095-98-6 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 151096-11-6 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, ethyl ester, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 151096-12-7 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-(2,4-difluorophenyl)-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

HCl

RN 151096-27-4 CAPLUS

1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-7-[1-(3-ethoxy-3-oxo-1-propenyl)octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl]-6-fluoro-1,4-dihydro-4-oxo-, [4aS-[1(E),4a.alpha.,7a.alpha.]]- (9CI) (CA INDEX NAME)

RN 151213-20-6 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 1-cyclopropyl-6-fluoro-1,4-dihydro-7-(octahydro-6H-pyrrolo[3,4-b]pyridin-6-yl)-4-oxo-, monohydrochloride, (4aS-cis)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

● HCl

09/833,914

ANSWER 27 OF 28 CAPLUS COPYRIGHT 2002 ACS

AN 1991:408619 CAPLUS

DN 115:8619

TI Synthesis of a new bridged diamine, 3,6-diazabicyclo[3.2.0]heptane: applications to the synthesis of quinolone antibacterials

AU Jacquet, Jean Pierre; Bouzard, Daniel; Kiechel, Jean Rene; Remuzon, Philippe

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DT Journal

LA English

OS CASREACT 115:8619

GΙ

AB Diprotected 3,6-diazabicyclo[3.2.0]heptane I has been prepd. by a highly efficient process, starting from pyrrolidine II. Debenzylation of I by catalytic hydrogenation, followed by condensation with 7-haloquinolone III (X = CH, R = H, R1 = F) or chloronaphthyridinone III (X = X, X = X) led to the the quinolone IV (X = X) and naphthyridinone IV (X = X) resp., which are potential antibacterials.

IT 134253-09-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (prepn. and N-deprotection and ester hydrolysis of)

RN 134253-09-1 CAPLUS

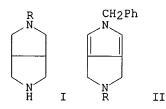
CN 1,8-Naphthyridine-3-carboxylic acid, 1-(1,1-dimethylethyl)-6-fluoro-1,4-dihydro-4-oxo-7-[6-(trifluoroacetyl)-3,6-diazabicyclo[3.2.0]hept-3-yl]-, ethyl ester (9CI) (CA INDEX NAME)

IT 134253-10-4P

RN 134253-10-4 CAPLUS

CN 1,8-Naphthyridine-3-carboxylic acid, 7-(3,6-diazabicyclo[3.2.0]hept-3-yl)-1-(1,1-dimethylethyl)-6-fluoro-1,4-dihydro-4-oxo- (9CI) (CA INDEX NAME)

ANSWER 28 OF 28 CAPLUS COPYRIGHT 2002 ACS 1983:488081 CAPLUS 99:88081 Synthesis and carbon-13 NMR study of 2-benzyl, 2-methyl, 2-aryloctahydropyrrolo[3,4-c]pyrroles and the 1,2,3,5tetrahydropyrrolo[3,4-c]pyrrole ring system ΑU Ohnmacht, Cyrus J., Jr.; Draper, Clyde W.; Dedinas, Robert F.; Loftus, Philip; Wong, J. J. Stuart Pharm. Div., ICI Americas Inc., Wilmington, DE, 19897, USA CS SO Journal of Heterocyclic Chemistry (1983), 20(2), 321-9 CODEN: JHTCAD; ISSN: 0022-152X DTJournal English LΑ OS CASREACT 99:88081 GΙ



Octahydropyrrolo[3,4-c]pyrroles I (R = CH2Ph, Ph, 3-MeOC6H4, 3-F3CC6H4) were prepd. in 5 steps from 1-benzylpyrrole-3,4-dicarboxylic acid. I (R = Me) was prepd. analogously in 6 steps from 1-methylpyrrole-3,4-dicarboxylic acid. Diborane redn. of 1-benzyl-N-methyl-1H-pyrrole-3,4-dicarboximide and 1,N-dibenzyl-1H-pyrrole-3,4-dicarboximide gave II (R = Me, CH2Ph), the first reported members of the 1,2,3,5-tetrahydropyrrolo[3,4-c]pyrrole ring system. A detailed study of the 13C-NMR shifts permitted a complete assignment for all compds. Mono- and disubstituted products produce a systematic effect on the shifts for the bicyclic ring systems which can be readily interpreted in terms of substituent chem. shifts. The effect of protonation at N produces a series of well defined chem. shifts for the octahydropyrrolo[3,4-c]pyrrole ring system.

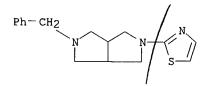
IT 86732-38-9P 86732-40-3P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (prepn. and carbon-13 NMR of)

RN 86732-38-9 CAPLUS

CM 1

CRN 86732-37-8 CMF C16 H19 N3 S



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CM 2

CRN 110-16-7 CMF C4 H4 O4

Double bond geometry as shown.

RN 86732-40-3 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(phenylmethyl)-5-(2-pyrimidinyl)-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

IT 86732-37-8P 86732-39-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (prepn. of)

RN 86732-37-8 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(phenylmethyl)-5-(2-thiazolyl)- (9CI) (CA INDEX NAME)

RN 86732-39-0 CAPLUS

CN Pyrrolo[3,4-c]pyrrole, octahydro-2-(phenylmethyl)-5-(2-pyrimidinyl)- (9CI) (CA INDEX NAME)